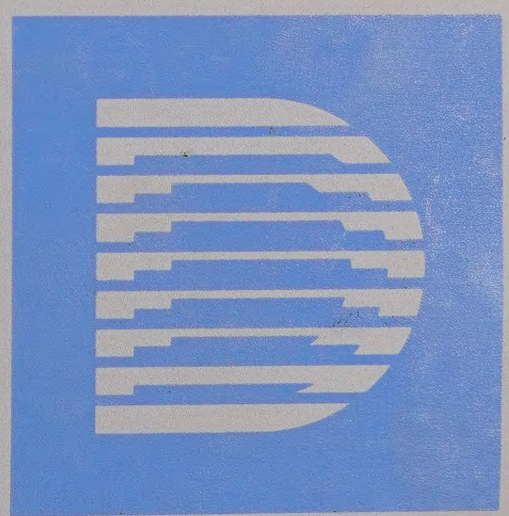


DIONEX

DIONEX

Dionex
Corporation
North Pointe Commons
9 East Stow Road
Marlton, NJ
08053-3118

Carolyn McGinnis
Service Coordinator
Eastern Region

609 596 0600
Fax 609 596 5358

DIONEX CORPORATION

AI-450 WORKSTATION

(Software Revision 3.31)

TRAINING COURSE

DIONEX CORPORATION
P.O. BOX 3603
SUNNYVALE, CA 94088-3603

(c) Copyright Dionex Corporation 1993
Document No. 034557-02
March 1993

Digitized by the Internet Archive
in 2025

https://archive.org/details/manualsplus_09474

Copyright

© 1993 DIONEX Corporation
All rights reserved worldwide.
Printed in the United States of America.

TRADEMARKS

1-2-3 Lotus, and Symphony are registered trademarks of Lotus Development Corporation.
Aldus and PageMaker are registered trademarks of Aldus Corporation.
dBase is a trademark of Ashton-Tate.
Foxy 200 is a trademark of Isco, Inc.
IBM PC/AT is a registered trademark of International Business Machines Corporation.
Microsoft Windows is a trademark, and Microsoft Excel, Microsoft Word, and MS-DOS are registered trademarks, of Microsoft Corporation.
WordPerfect is a registered trademark of WordPerfect Corporation.
WordStar is a registered trademark of WordStar International Incorporated.

All other trademarks and registered trademarks are the property of their respective owners.

All rights reserved. No part of this publication may be copied or distributed, transmitted, transcribed, stored in a retrieval system, or transmitted into any human or computer language, in any form or by any means, electronic, mechanical, magnetic, manual, or otherwise, or disclosed to third parties without the express written permission of DIONEX Corporation, 1228 Titan Way, Sunnyvale, California 94088-3603.

COURSE OBJECTIVES

Day 1 Computer Basics and Getting Started with AI-450

1. Describe the different parts of a computer and explain the "booting" process.
2. Diagram the hard disk directory structure on your computer
3. Manipulate a Window by sizing, dragging, minimizing, and maximizing.
4. Customize the colors on your computer screen, and fine-tune your mouse using the Windows Control Panel program.
5. Configure your AI-450 software for your chromatographic system.
6. Coordinate instrument control and data acquisition using the METHOD program.
7. Collect chromatographic data from a Dionex instrument using the RUN program.
8. Interpret the resulting report and make necessary changes to the METHOD file in order to acquire the chromatographic data properly.
9. Run multiple samples or standards using the SCHEDULE program.
10. Archive data files or delete data files not needed and then perform periodic disk maintenance to speed up future processing.

COURSE OBJECTIVES (Continued)

Day 2 Advanced Data Manipulation and Customizing Reports.

1. Improve chromatographic integration using the OPTIMIZE program.
2. Process multiple data files using the BATCH program.
3. Obtain statistics on replicate samples or standards using BATCH.
4. Evaluate calibrations using the CALPLOT program.
5. Compare multiple data files using the VIEW program and export the graphics for report writing.
6. Export chromatograms and chromatographic reports to other Windows programs.
7. Create professional-looking reports using the graphics and text imported into these Windows programs.
8. Manipulate system programs to create a customized startup protocol.

AI-450 COURSE OUTLINE

I Introduction and Computer Basics
- A. Course Objectives and Outline
- B. Intro to Computer Hardware and a Peek inside the Computer.
- C. What Happens When I Turn On the Computer?
- D. Computer Software - Programs vs. Files
- E. RAM vs ROM vs Disk Memory
- F. Directory Structure (Exercise 1)

II DOS and WINDOWS
- A. What is DOS and What does it do?
- B. What is the WINDOWS program and Why do we use it?
- C. Operating Modes of WINDOWS 3.1
- D. Anatomy of a Window
- E. Manipulation of the Mouse and the Window
- F. Control Panel
- G. File Manager and File Organization
- H. Dialog Boxes and Inputting into WINDOWS (Exercise 2)

III Advanced WINDOWS Features
- A. Special Programs
  1. Notepad and Write
  2. Clipboard and PaintBrush
- B. Exporting from AI-450 Programs (Windows Exercise)
- C. Arranging Icons with Program Manager
- D. Editing AUTOEXEC.BAT and CONFIG.SYS

IV Getting Started with AI-450
- A. MAINMENU and HELP (Exercise 3)
- B. CONFIGURE (Exercise 4)
- C. Coordinating data collection with METHOD (Exercise 5)
- D. Collecting Data with RUN (Exercise 6)
- E. Running Multiple Samples Using SCHEDULE (Exercise 7)

V Interpreting the Report and Archiving the Data
- A. What information is in the report?
- B. Remedies for Ailing Chromatograms using METHOD
- C. Deleting or Archiving Data Files
- D. Disk Maintenance (Exercise 8)

VI OPTIMIZE-ing the Integration
- A. Getting Started with a Data File
- B. Editing the Method File
- C. Operations of OPTIMIZE
- D. What to try first - Initial Values
  1. Measuring Peak Widths
  2. Autothreshold measurements
- E. What to try next - Data Events
  1. Description of Common Events
  2. How to enter and test them
- F. The last resort - Manual Baselines!
- G. Adjusting Named Peaks
- H. Customizing Graphics and Printout
- I. Exporting and Copying (Exercise 9)

VII Optimizing Many Data Files with BATCH
- A. Browsing and Deleting Data Files
- B. Building or Modifying a BATCH Schedule
- C. Processing and Export Options
- D. Batch Settings File
- E. Controls and Priority

VIII Viewing Calibrations with CALPLOT
- A. Editing the Components or the Calibration
- B. Use of the "Calculator"
- C. Using BATCH and CALPLOT (Exercise 10)

IX Viewing Multiple Chromatograms with VIEW
- A. Previewing and Selecting Files
- B. Changing the Viewing Format
- C. Exporting (Exercise 11)

X The DATAMATH program and When it is Used

XI Customizing Reports with FORM (Optional)

AI-450 TRAINING COURSE

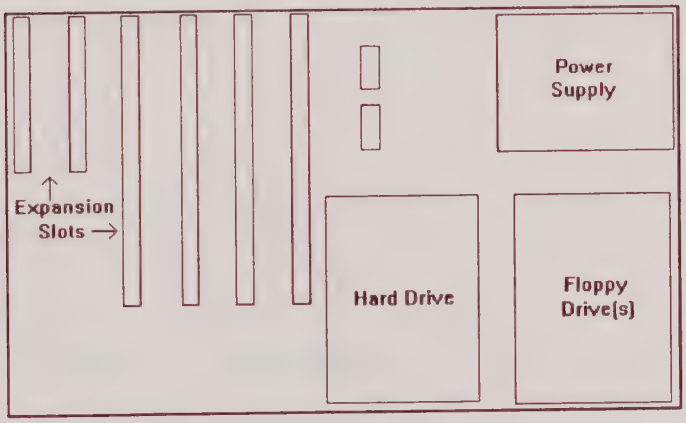
I Introduction and Computer Basics

A. Course Objectives and Outline

B. Introduction to Computer Hardware and a Peek Inside the CPU

1. Hardware
   - Computer
   - Hard Drive
   - Floppy Drive(s)
   - Monitor
   - Keyboard
   - Mouse

View from the Top



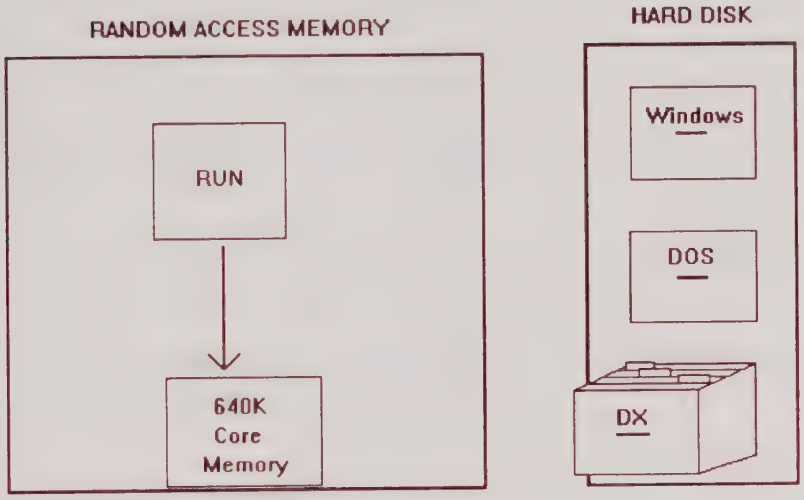
C. What Happens When the Computer Powers Up?

- Checks Memory and Hardware and Beeps when done.
- Loads DOS into memory from floppy or hard drive.
- Locates CONFIG.SYS and performs commands
- Runs AUTOEXEC.BAT

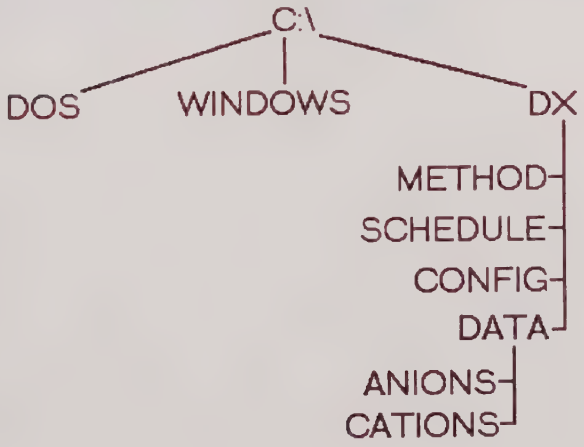
D. Computer Software

- Programs (*.BAT, *.EXE, or *.COM)
- Files (examples: *.TXT, *.BMP, *.D01)

E. RAM vs. ROM vs. Disk Memory



F. Disk Directory Structure



EXERCISE 1

A. In Main Menu press [Ctrl], [Alt], and [Del] simultaneously (This is called "warm booting" or "soft resetting" your computer). What happens?

_____

_____

_____

How is this different from turning the computer on?

_____

_____

_____

B. Put a floppy disk supplied by the instructor into the A drive of the computer and warm boot the computer again. What happens?

_____

_____

_____

This message would not appear if the disk had a program on it called COMMAND.COM. This file makes the disk a "System Disk" and the computer can "boot" off of it. This is the way you would start your computer if there was something wrong with your hard disk.

II DOS and WINDOWS (VERSION 3.1)

A. What is DOS and What does it do?

- DOS stands for Disk Operating System.

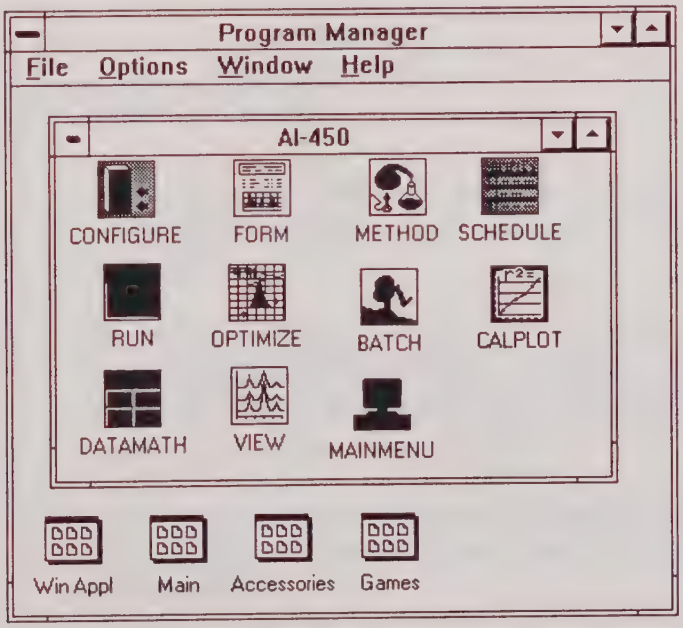
- DOS is a system program (MS-DOS is Microsoft's version and PC-DOS is IBM's version) as opposed to an application program.

- DOS controls every part of the computer system so other programs don't have to.

- Disk Operating Systems manage disks and disks files.

- Commands tell DOS what to do.
  e.g. DIRectory, REName, FORMAT

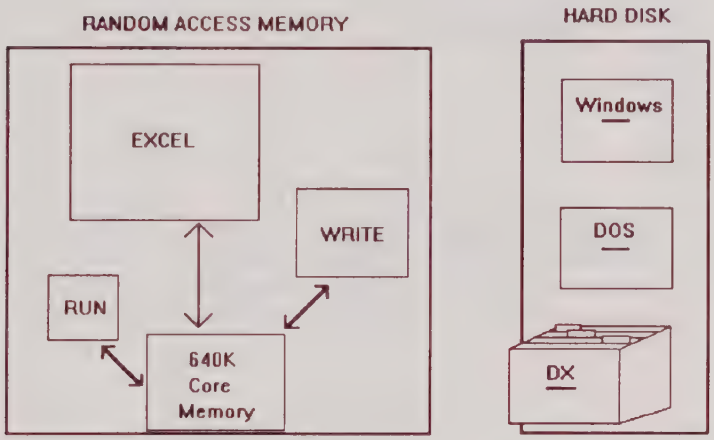
B. What is the WINDOWS program and Why do we use it?



- WINDOWS is a graphical environment which allows you to run DOS and other commands by selecting from a menu.

- WINDOWS allows you to use a mouse instead of the keyboard to give the computer commands.

- WINDOWS lets you work with more than one application at a time.



- Dionex uses WINDOWS as the operating environment to make operating your system and collecting data easier and more FUN!

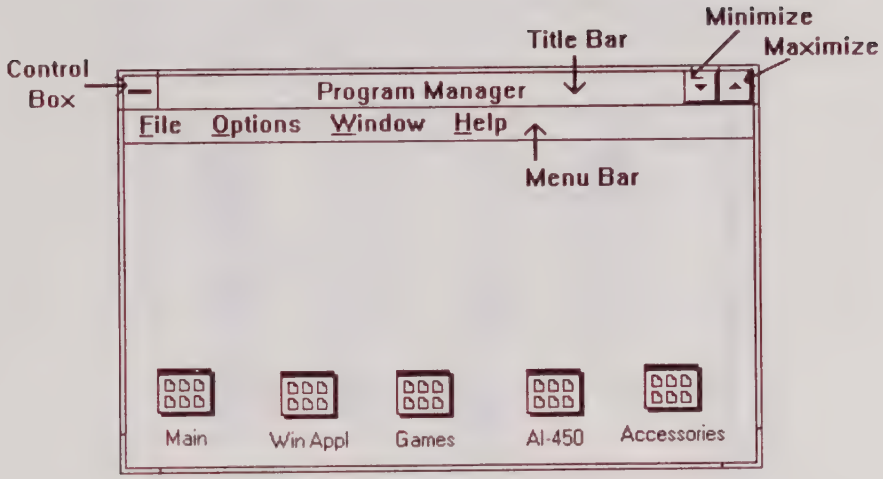
C. Operating Modes of WINDOWS 3.1

- **Standard Mode** is the basic operating mode which provides access to extended memory and enables you to switch between applications.

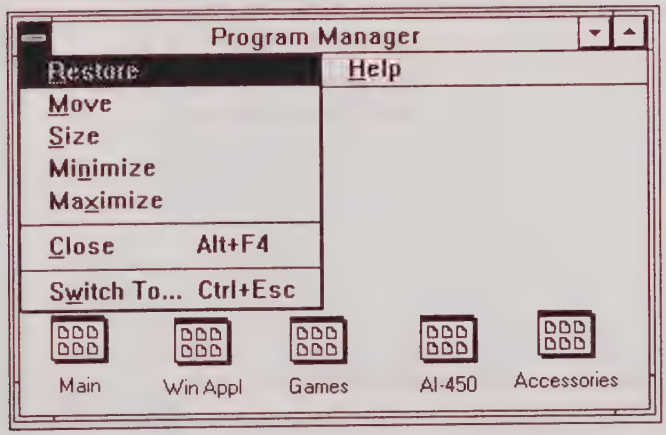
- **386 Enhanced Mode** allows the use of virtual memory capabilities of the 386 and higher processors. In the enhanced mode, applications have access to more memory than is physically available on your system.

- Using the command **WIN** without a designation allow Windows to run in whatever mode is appropriate for the hardware configuration.

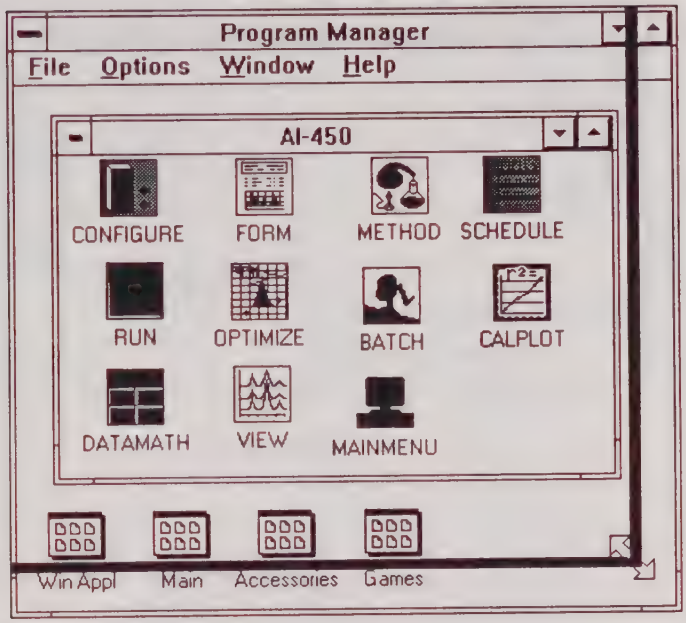
D. Anatomy of A Window



1. Title Bar
2. Menu Bar
3. Maximize and Minimize
4. Control Box gives access to manipulation commands from the keyboard instead of the mouse.



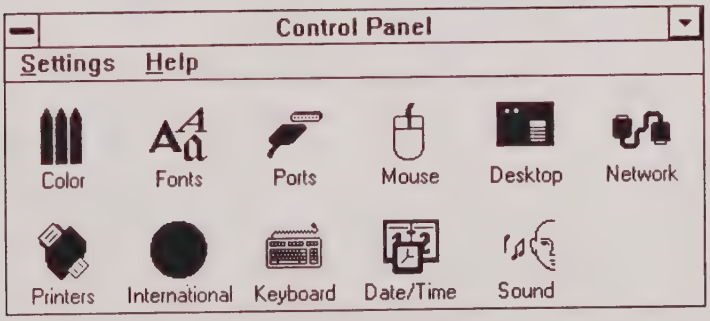
E. Manipulation of the Mouse and the Window



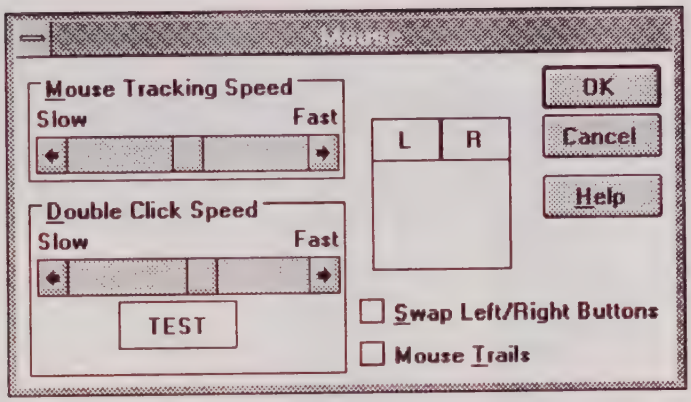
1. Mouse Operations
   - Click
   - Click and Drag
   - Double Click

2. Window Manipulations
   - Maximize and Minimize
   - Moving
   - Sizing
   - Closing and Restoring

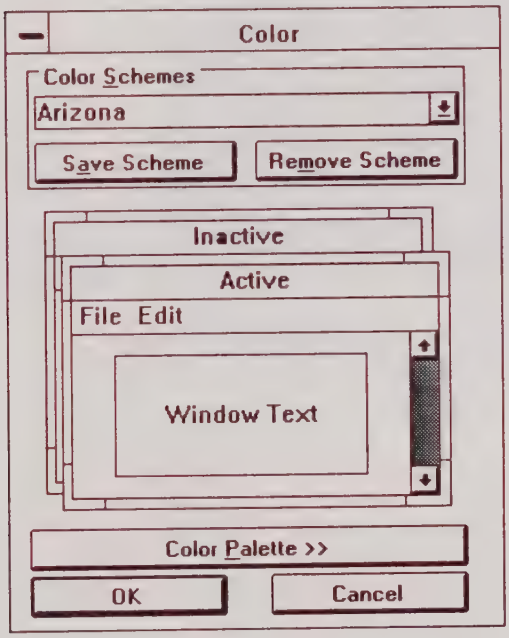
F. Control Panel



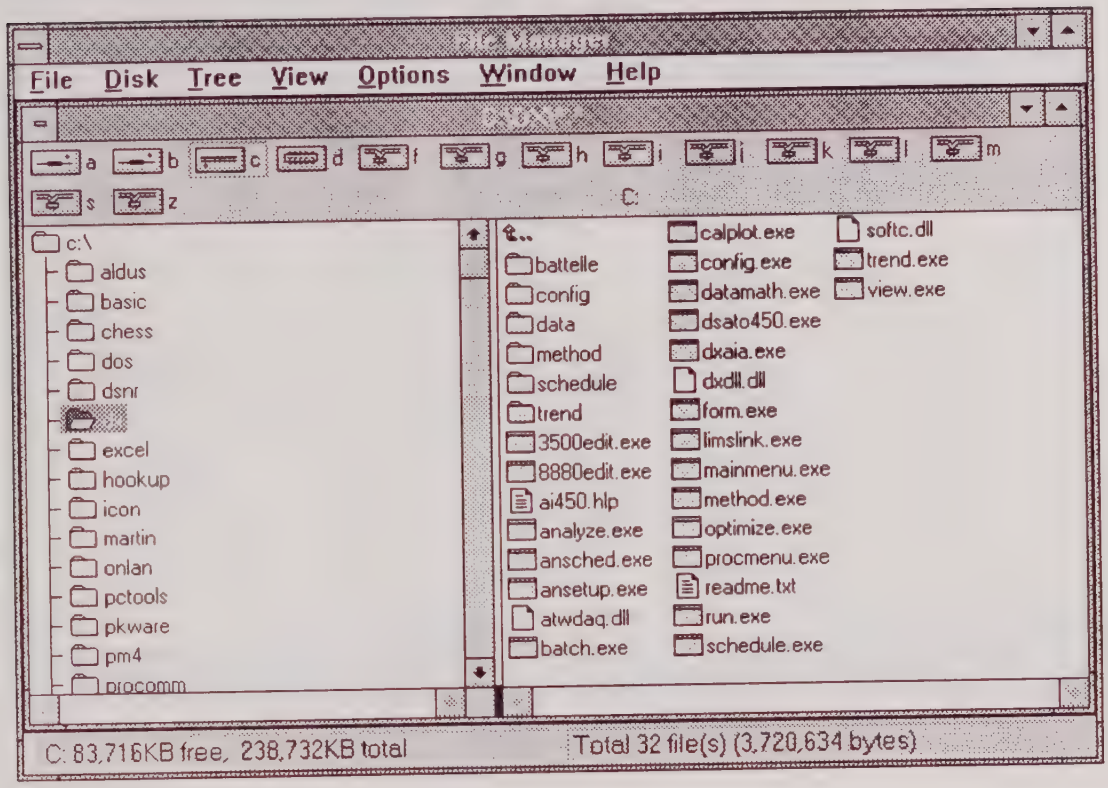
1. Mouse Settings



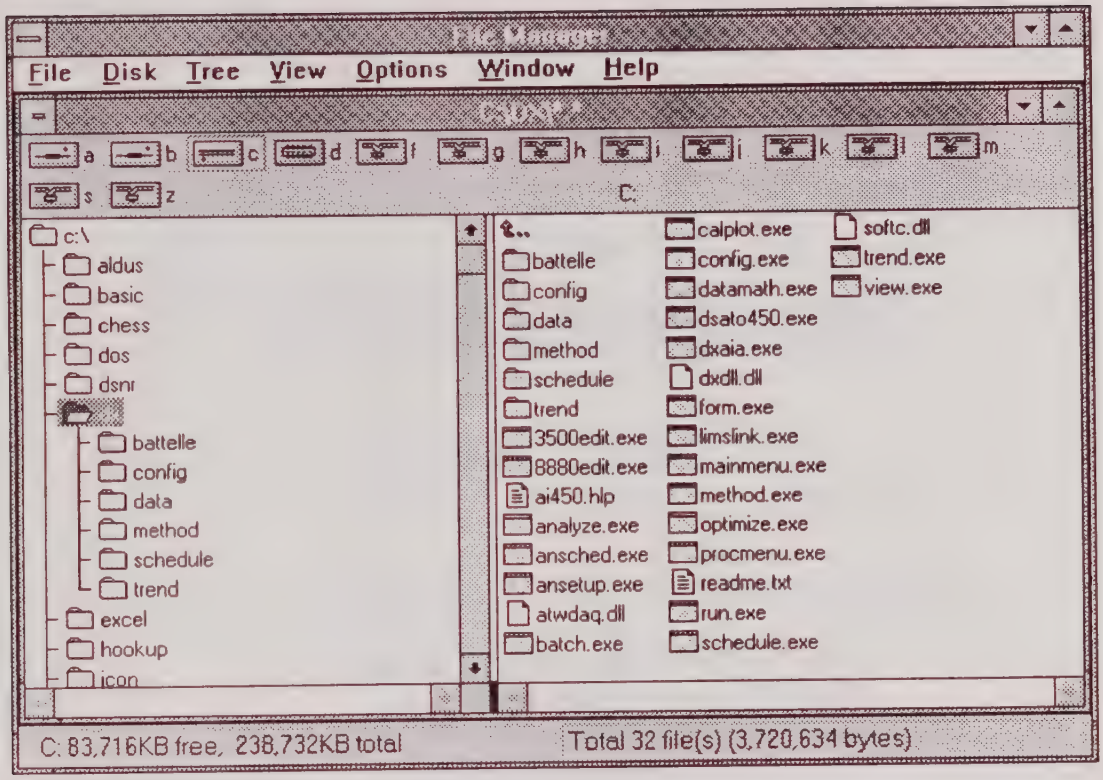
2. Adjusting Screen Colors

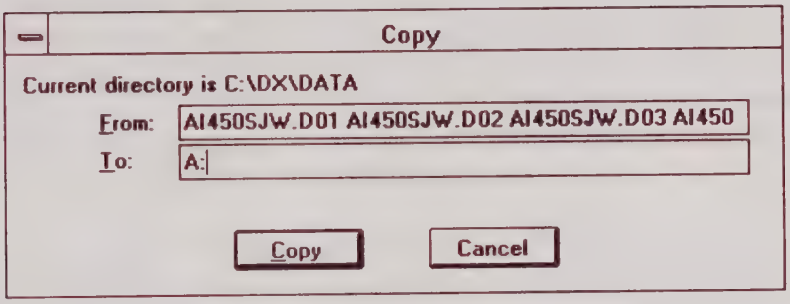


G. File Manager and File Organization



- By double-clicking on the subdirectory "DATA", you can see the files in that directory:


File Manager
File Disk Tree View Options Window Help
C:*.*
a b c d f g h i j k l m
s z
C:
c:\
aldus
basic
chess
dos
dsnr
battelle
config
data
method
schedule
trend
excel
hookup
icon
battelle
config
data
method
schedule
trend
3500edit.exe
8880edit.exe
ai450.hlp
analyze.exe
ansched.exe
ansetup.exe
atwdaq.dll
batch.exe
calplot.exe
config.exe
datamath.exe
dsato450.exe
dxaia.exe
dxdll.dll
form.exe
limslink.exe
mainmenu.exe
method.exe
optimize.exe
procmenu.exe
readme.txt
run.exe
schedule.exe
softc.dll
trend.exe
view.exe
C: 83,716KB free, 238,732KB total
Total 32 file(s) (3,720,634 bytes)



1. You Can Use <TAB> or the Mouse to Change Fields

2. Telling the Computer Which Files to Copy
   a. Path Designation (e.g. C:\DX\DATA)
   b. * Wild Card designates up to 8 characters.
   c. ? Wild Card designates one character
   d. Point and Click with the Mouse while holding down [Ctrl] or [Shift]

3. Clicking on the "Copy" button invokes the command.

4. Other File Menu Commands
   a. **Move** files from one directory to another.
   b. **Delete** files from the directory
   c. **Rename** one file at a time
   d. **Create Directory** under another directory.

EXERCISE 2

A. From the DOS screen (dark screen except for text), type DIR at the prompt (this will look something like "C:\DX>"). What you see being listed on the screen are the files in that particular directory. These may be too numerous to be listed on only one screen, so they may scroll by too quickly to be read. You can list only the names of the files, which may fit on one screen, by typing the option "**/w**" after the DIR command (i.e "DIR/w"). You can have the listing pause after one screen by typing the option "**/p**" after the DIR command. Try one of these command options with the DIR command.

B. Start the WINDOWS program by typing the **WIN** command at the prompt. After the PROGRAM MANAGER window is displayed, investigate the mode WINDOWS is running by clicking the mouse on the "HELP" menu and then clicking on the "About Program Manager..." command.

In what mode is WINDOWS running on your computer?

_____

The memory message displayed in the "ABOUT" Window refers to the free RAM available to run programs. How much RAM is available on your computer? _____

C. Try changing the size of the Program Manager window by clicking and dragging with the mouse on the borders of the window. How narrow can you make the window? _____
How short can you make the window? _____
Minimize and **maximize** the Program Manager window and then "RESTORE" it to it's original size, using the up and down arrows in the upper right-hand corner of the window. To restore a minimized window (also known as an "**Icon**"), you can double click on the icon. Minimizing a program is a convenient way to "clean up" a cluttered computer screen (also known as the **desktop**) to more easily access programs you are working on without ending (or **closing**) the program.

D. Use the **Mouse** and **Colors** options in the **Control Panel** program to set the mouse acceleration and double clicking speed to your preference and to adjust the computer screen colors to your liking.

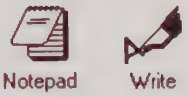
E. Using the **Create Directory** command in the File Menu of Program Manager, create the directory C:\DX\DATA\CLSANION.

F. Obtain a floppy disk from the instructor. Use the mouse or multiple-character wildcards to copy the AI-450 class data files (AI450*.*) files from the floppy disk to the C:\DX\DATA\CLSANION directory.

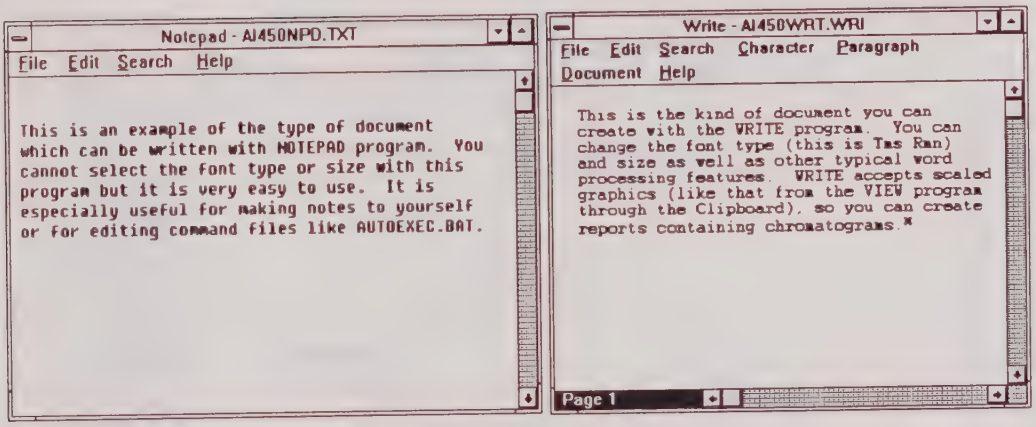
III Advanced WINDOWS Features

A. Special Programs

1. Notepad and Write

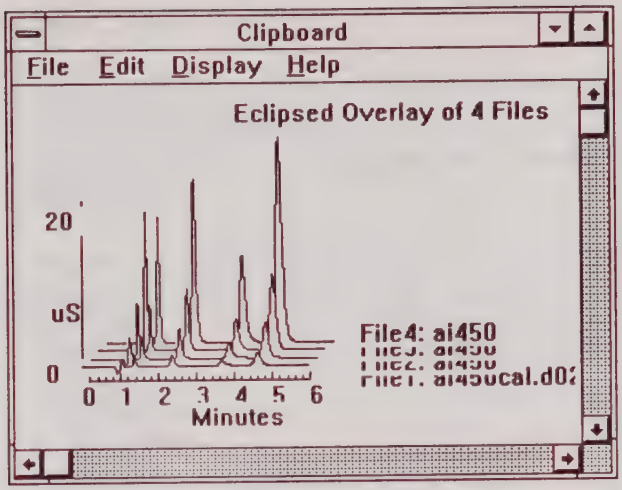


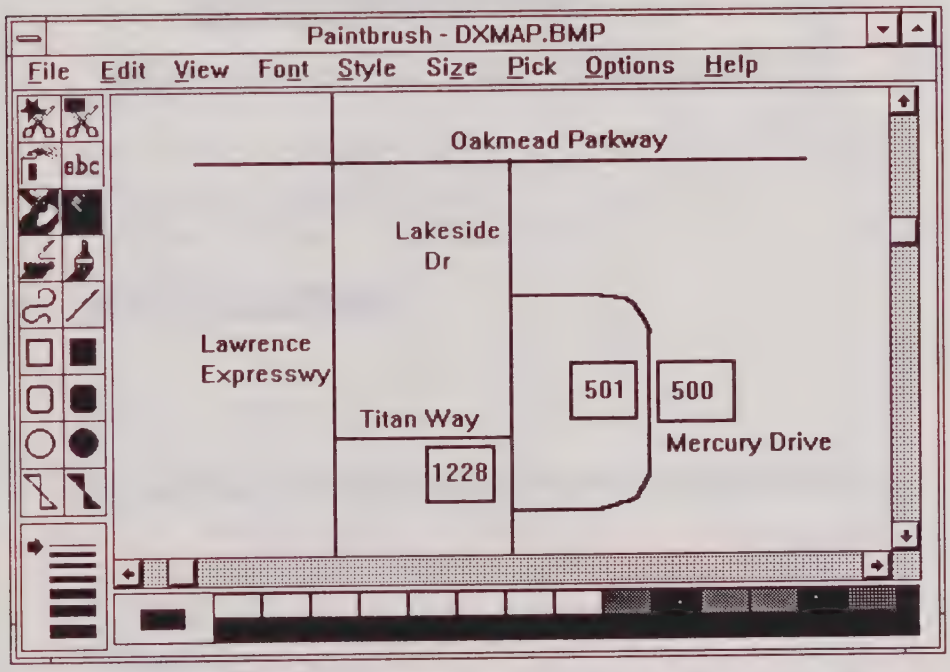
- These two are simple word processing programs with limited capabilities.


Notepad - AI450NPD.TXT
File Edit Search Help
This is an example of the type of document which can be written with NOTEPAD program. You cannot select the font type or size with this program but it is very easy to use. It is especially useful for making notes to yourself or for editing command files like AUTOEXEC.BAT.
Write - AI450WRT.WRI
File Edit Search Character Paragraph
Document Help
This is the kind of document you can create with the WRITE program. You can change the font type (this is Tms Rmn) and size as well as other typical word processing features. WRITE accepts scaled graphics (like that from the VIEW program through the Clipboard), so you can create reports containing chromatograms.
Page 1

2. Clipboard and Paintbrush

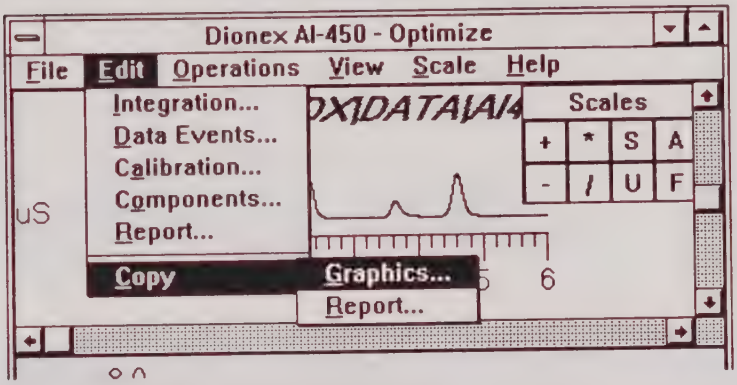
- these two programs allow you to create and manipulate graphics. Paintbrush can be used to create or modify graphic files known as BIT MAPS. The Clipboard program is like a parking place for graphics or text. This is where pictures or text goes when you "Cut" or "Copy" them within other programs.

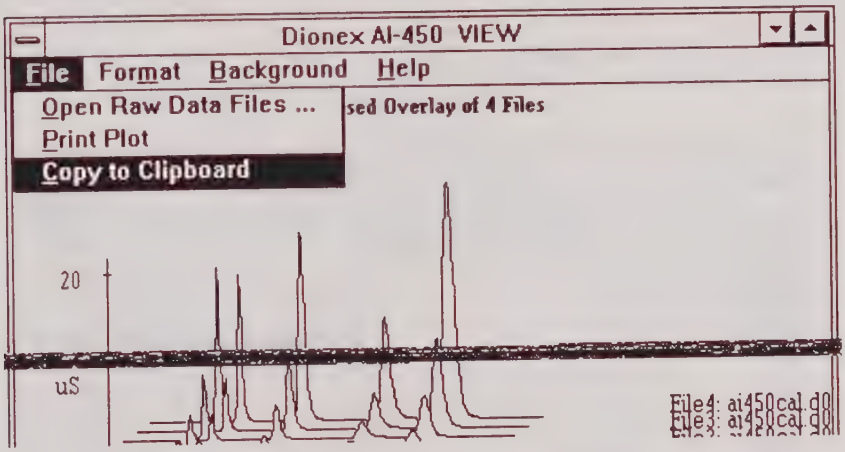

Clipboard
File Edit Display Help
Eclipsed Overlay of 4 Files
20
uS
0
0 1 2 3 4 5 6
Minutes
File4: ai450

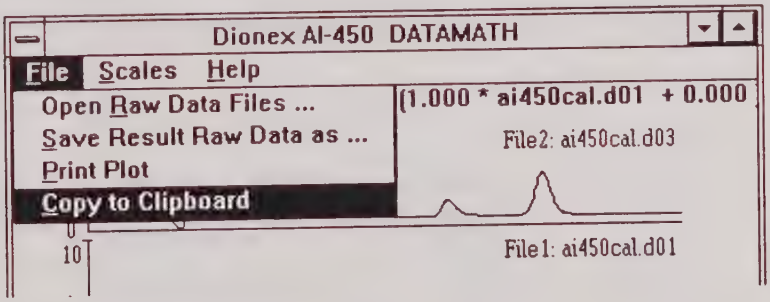

Paintbrush - DXMAP.BMP
File Edit View Font Style Size Pick Options Help
Oakmead Parkway
Lakeside
Dr
Lawrence
Expresswy
Titan Way
1228
501
500
Mercury Drive

B. Exporting from AI-450 Programs

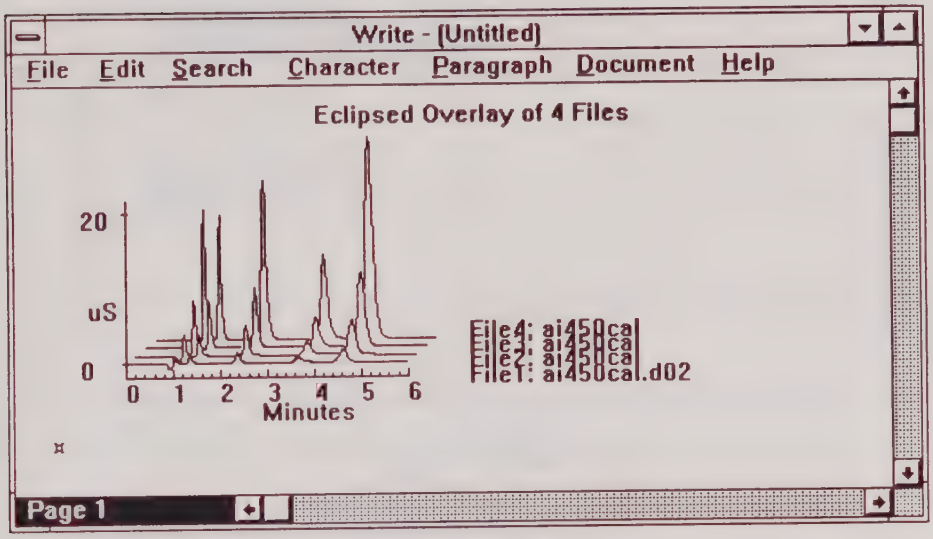
1. Copying to the Clipboard can be done in OPTIMIZE, VIEW and DATAMATH programs.
2. In OPTIMIZE you can copy either the chromatogram or the report to the clipboard.



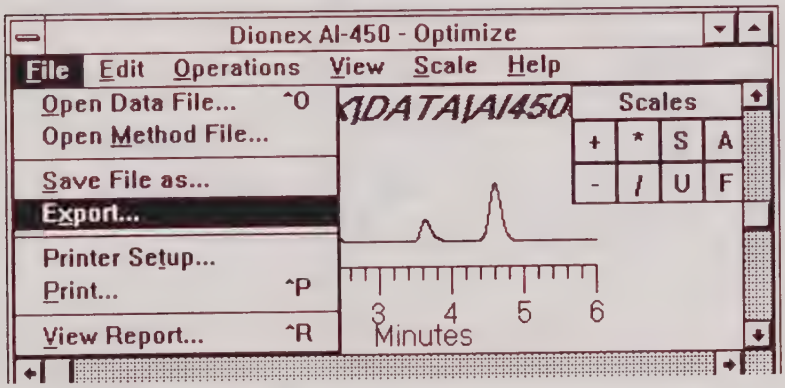


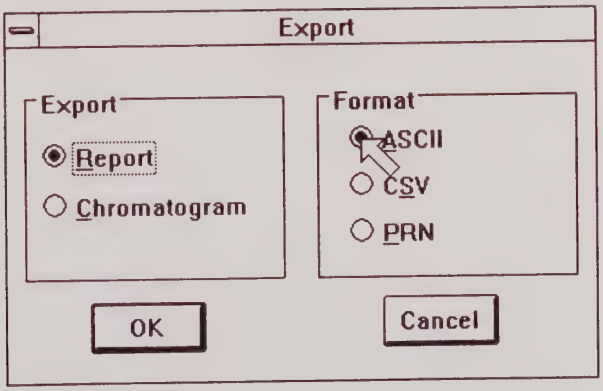


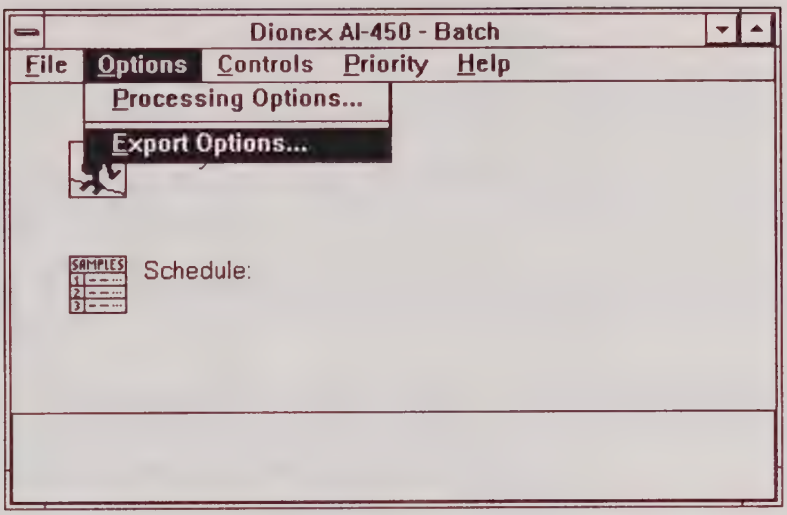
3. From the Clipboard, these can be "Pasted" into other programs, like Write.

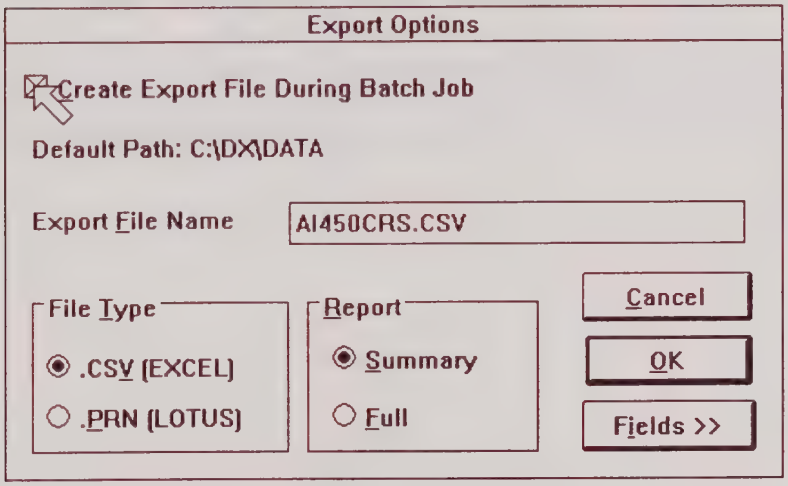


4. Exporting directly into files compatible with other programs can be done from OPTIMIZE, and BATCH.



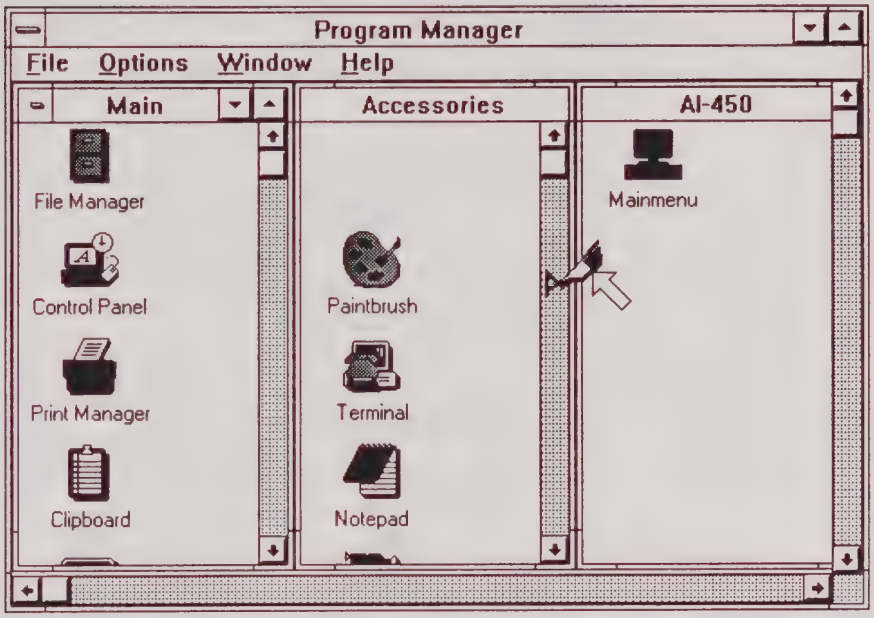



Dionex AI-450 - Batch
File
Options
Controls
Priority
Help
Processing Options...
Export Options...
SAMPLES
Schedule:

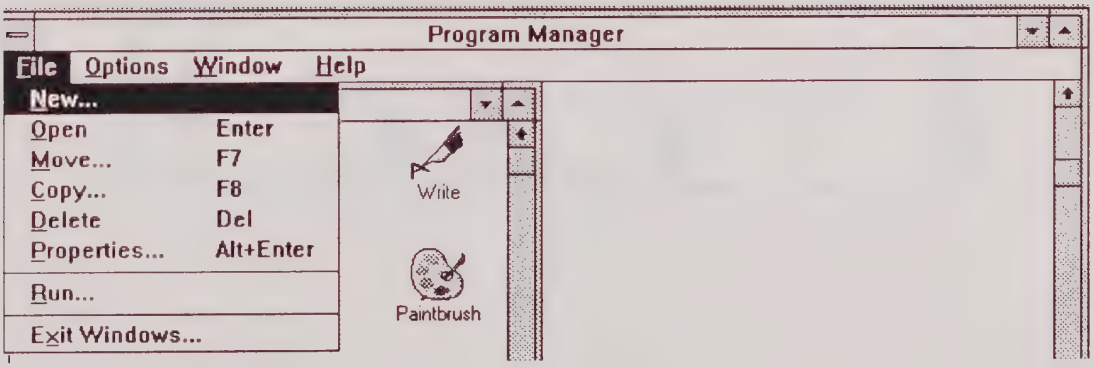

Export Options
Create Export File During Batch Job
Default Path: C:\DX\DATA
Export File Name
AI450CRS.CSV
File Type
.CSV (EXCEL)
.PRN (LOTUS)
Report
Summary
Full
Cancel
OK
Fields >>

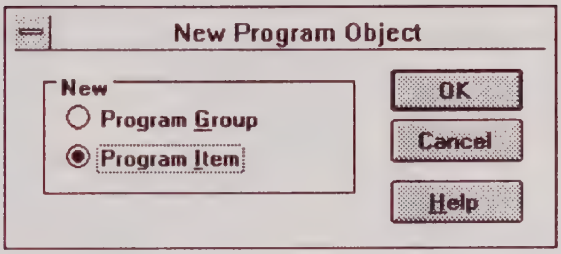
C. Arranging Icons with Program Manager

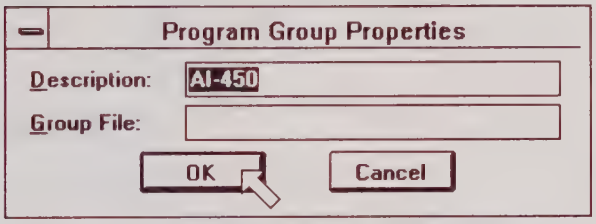
1. By clicking and dragging, you can organize the icons within the Program Manager groups in any way you'd like.

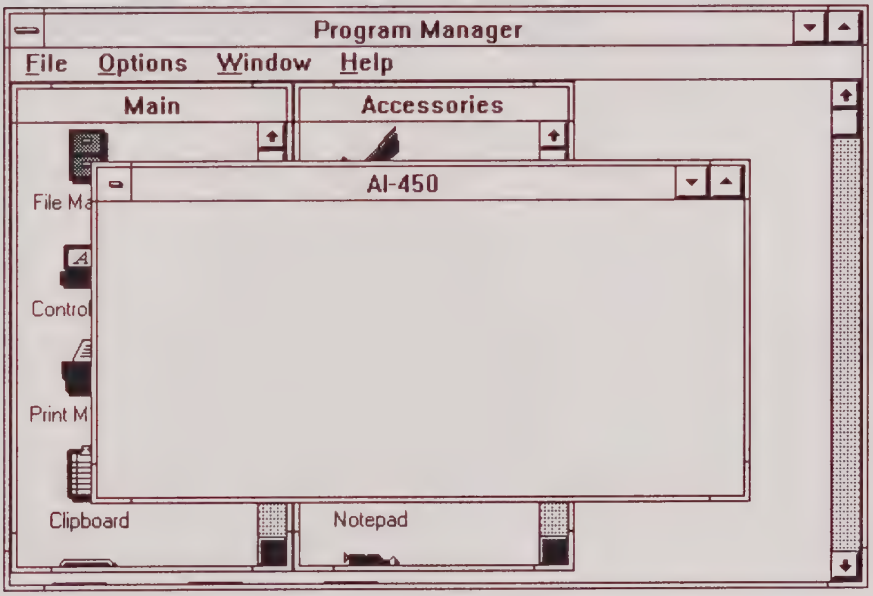


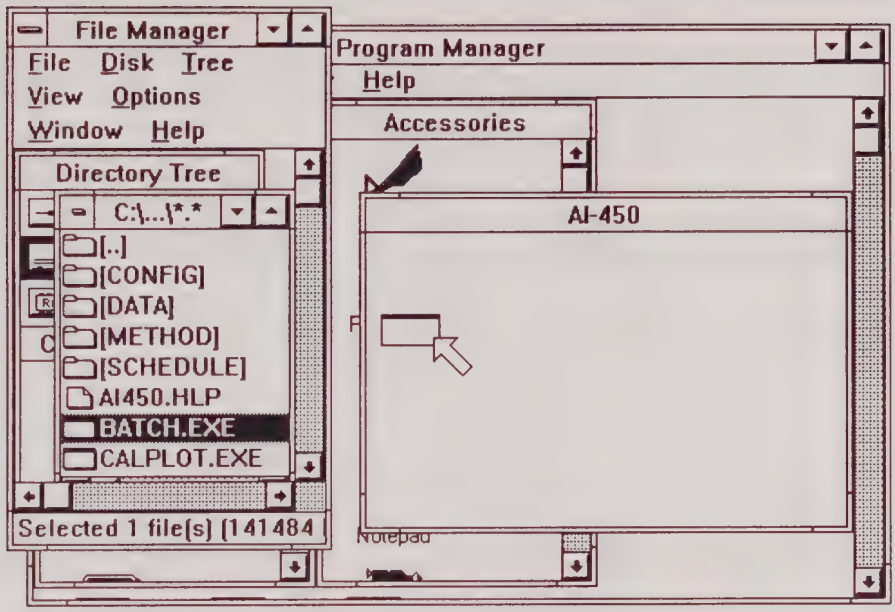
2. You can also create new groups in the Program Manager, by clicking and dragging programs from the File Manager into the new group.

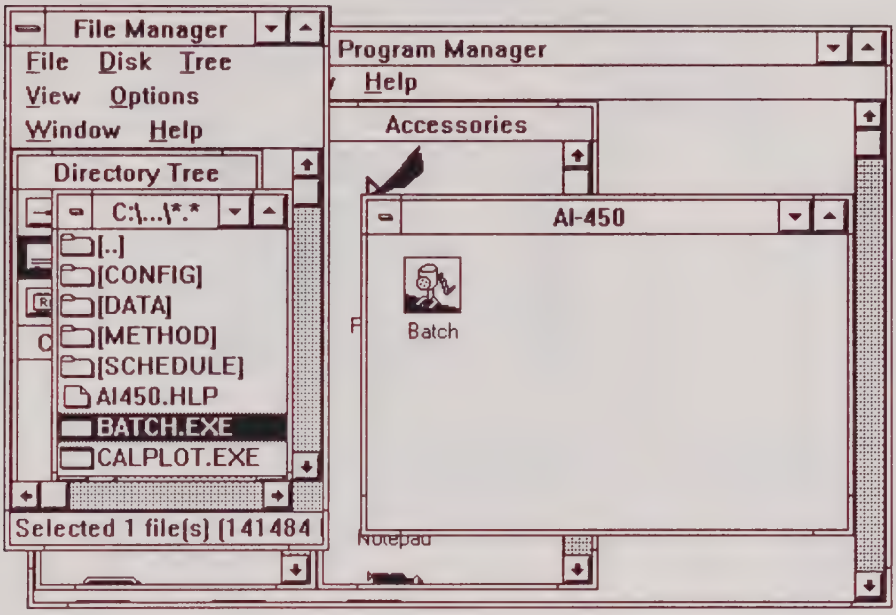



New Program Object
New
Program Group
Program Item
OK
Cancel
Help


Program Group Properties
Description:
AI-450
Group File:
OK
Cancel

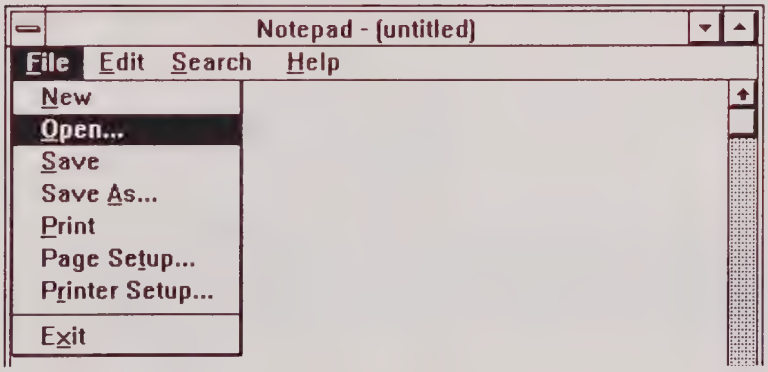

Program Manager
File
Options
Window
Help
Main
Accessories
AI-450
File Ma
Control
Print M
Clipboard
Notepad

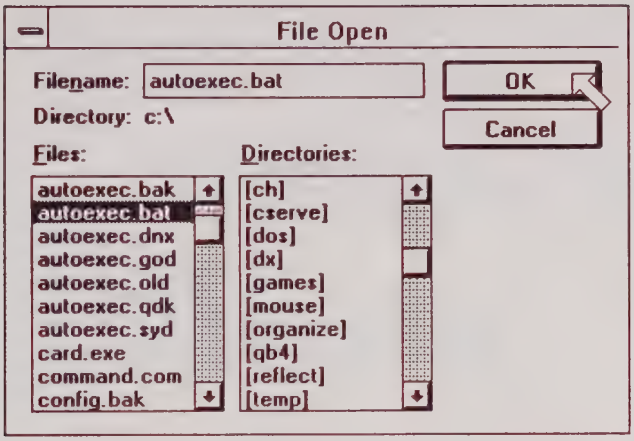

File Manager
File Disk Tree
View Options
Window Help
Directory Tree
C:\...*.*
[..]
[CONFIG]
[DATA]
[METHOD]
[SCHEDULE]
AI450.HLP
BATCH.EXE
CALPLOT.EXE
Selected 1 file(s) (141484
Program Manager
Help
Accessories
AI-450
Notepad

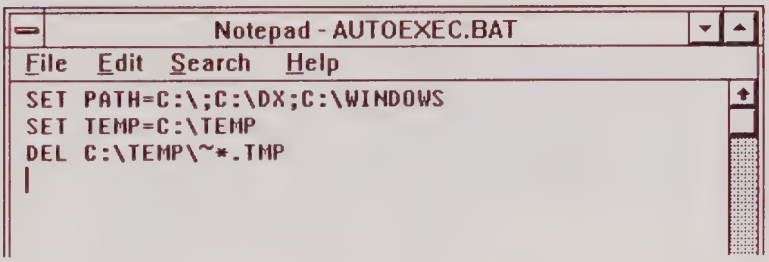


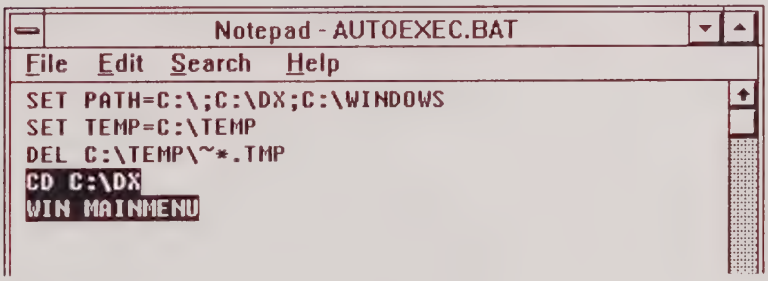
D. Editing AUTOEXEC.BAT and CONFIG.SYS

1. The AUTOEXEC.BAT file is the command file which dictates which commands are run when you boot your computer. It can be modified to run any programs you want when your computer is booted. As an example, let's add the commands to start Windows and run MainMenu in the DX directory upon bootup:





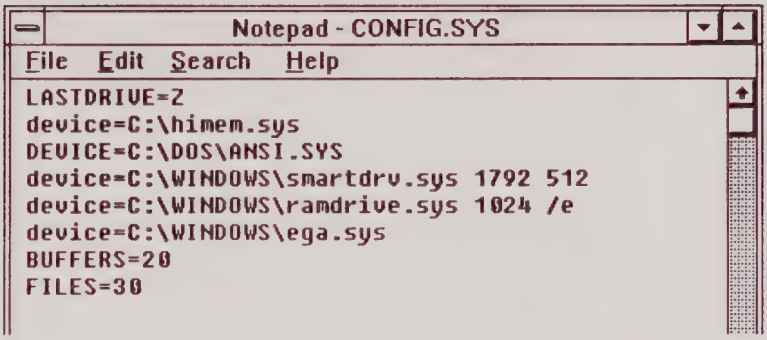




2. You would then save this file as "AUTOEXEC.BAT" and reboot the computer to see the effect.

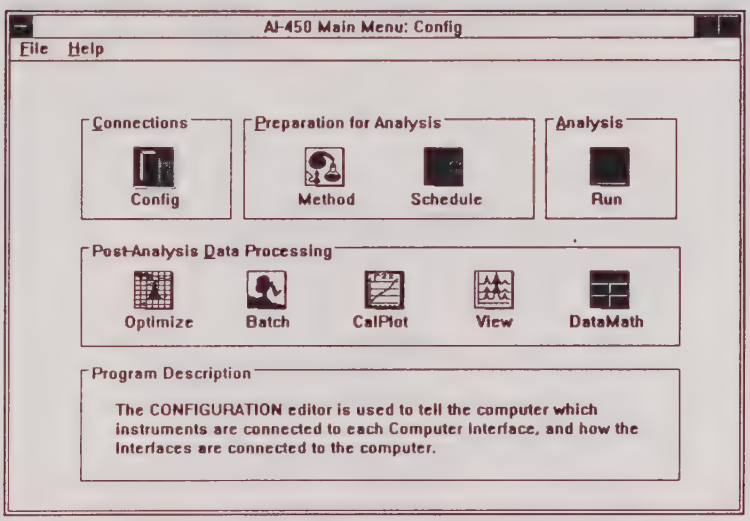
3. The AUTOEXEC.BAT was created when Windows was loaded on your computer and was modified when the AI-450 software was loaded. Usually the file does not need to be modified, but it is easy to do if you want to.

4. The CONFIG.SYS file is a file that contains information on the configuration of your computer, both hardware and software. A typical CONFIG.SYS file looks like this:

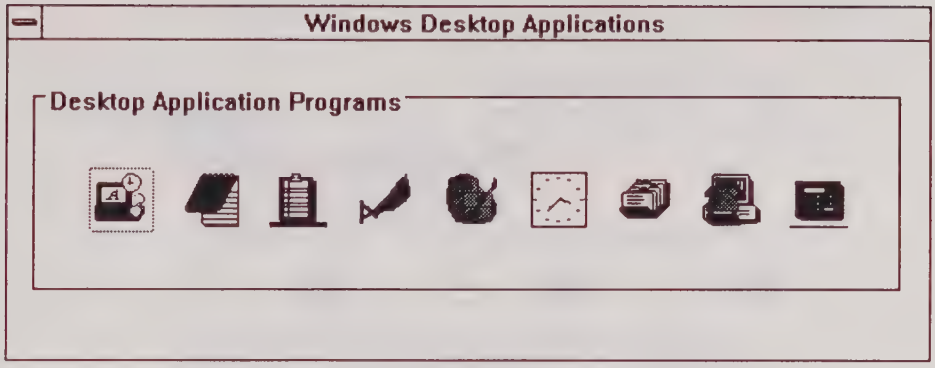


5. The CONFIG.SYS file is also created when Windows is loaded on your computer and modified (if necessary) when the AI-450 software is loaded. It is usually **NOT** necessary to change this file, but if you need to, it's just as easy as changing the AUTOEXEC.BAT file. Refer to your Windows manual for more details on the CONFIG.SYS file.

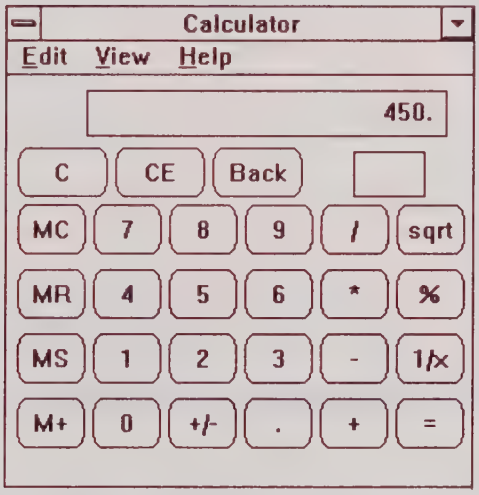
A. MAINMENU and HELP



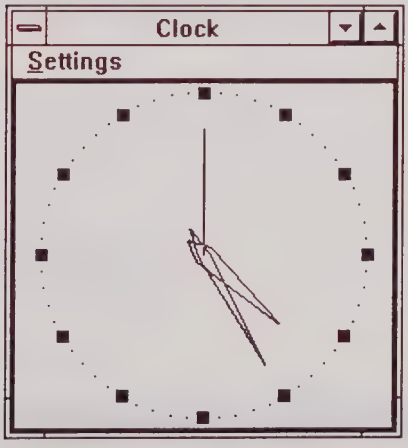
1. The text at the bottom of the window describes what each program does.
2. Start the program by double-clicking on the Icon.
3. Access WINDOWS applications from the File Menu.



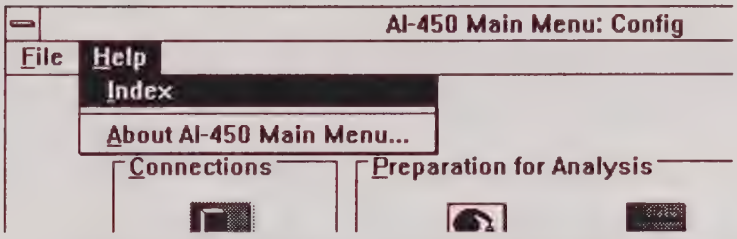
a. Control Panel (Discussed previously)
b. Calculator is for on-screen math help.

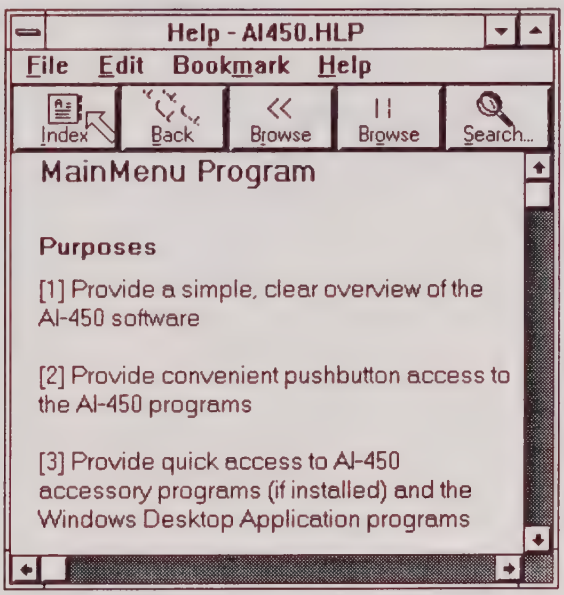


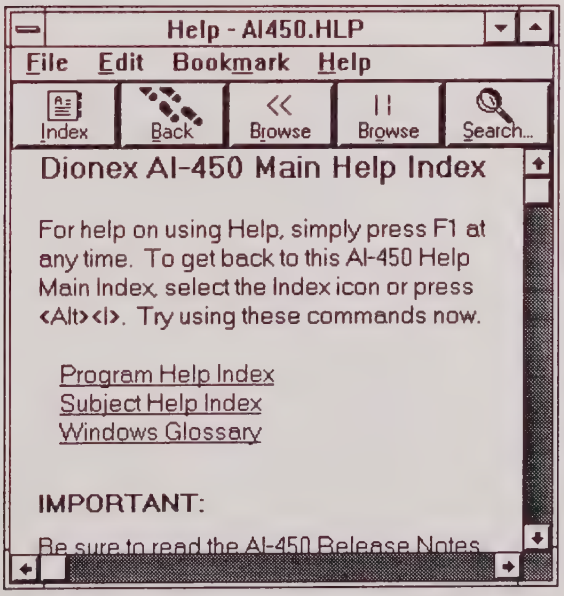
c. Clock is an on-screen timepiece.



4. Access the AI-450 Help Program from the Help Menu




Help - AI450.HLP
File Edit Bookmark Help
Index
Back
Browse
Browse
Search...
MainMenu Program
Purposes
[1] Provide a simple, clear overview of the AI-450 software
[2] Provide convenient pushbutton access to the AI-450 programs
[3] Provide quick access to AI-450 accessory programs (if installed) and the Windows Desktop Application programs


Help - AI450.HLP
File Edit Bookmark Help
Index
Back
Browse
Browse
Search...
Dionex AI-450 Main Help Index
For help on using Help, simply press F1 at any time. To get back to this AI-450 Help Main Index, select the Index icon or press <Alt><I>. Try using these commands now.
Program Help Index
Subject Help Index
Windows Glossary
IMPORTANT:
Be sure to read the AI-450 Release Notes

EXERCISE 3

A. Start the AI-450 MAINMENU program by double-clicking on it's Icon.

B. Read the short description of the CONFIG and METHOD programs by clicking once on the program icon - the description appears in the lower portion of the MAINMENU window.
What does a method file contain? _____

C. Run the CALCULATOR program from the MAINMENU File menu.
What is the square root of 987654? (to 4 significant fiqures)

_____

D. Start the AI450 Help from the MAINMENU Help menu. Using the mouse, select "Windows" under "Related Topics" and then select "Windows Glossary". What is the definition of "Active Window"?

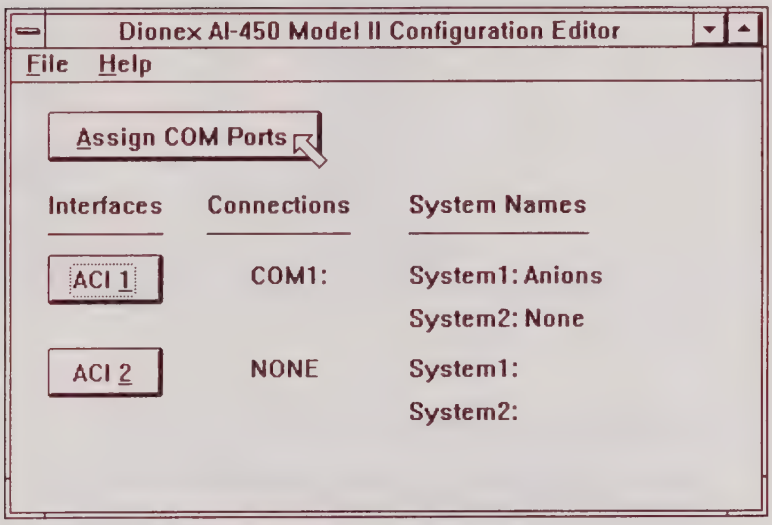
_____

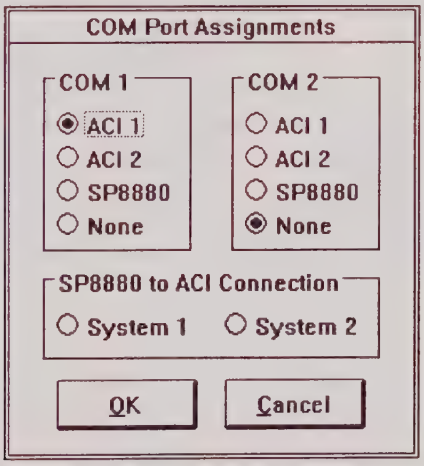
_____

B. CONFIGURE

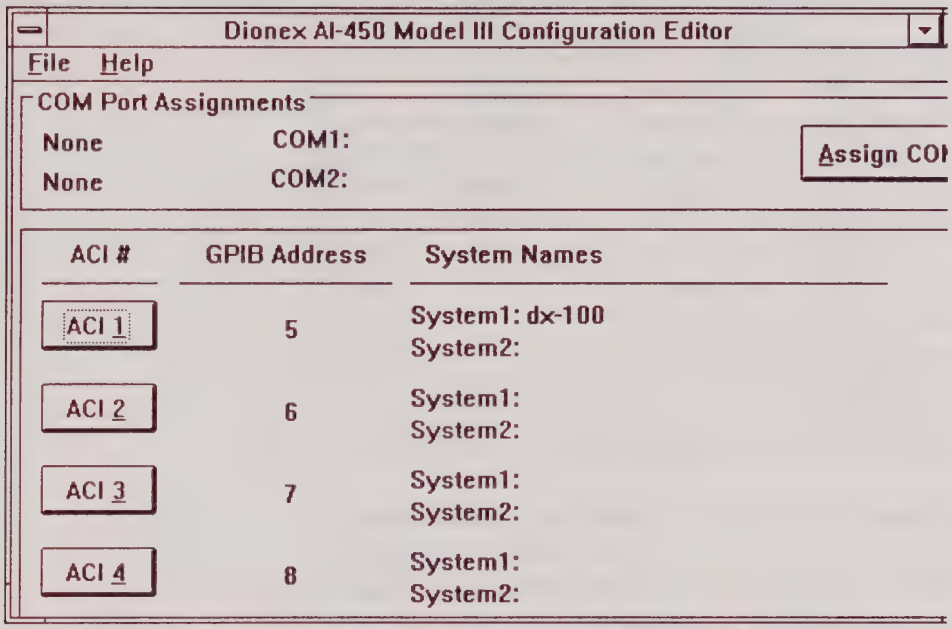
1. CONFIGURE Tells the Computer What is Connected to the Advanced Computer Interface (ACI).

    a. Assign Com Port(s) to Communicate with ACI(s) for Model I or II

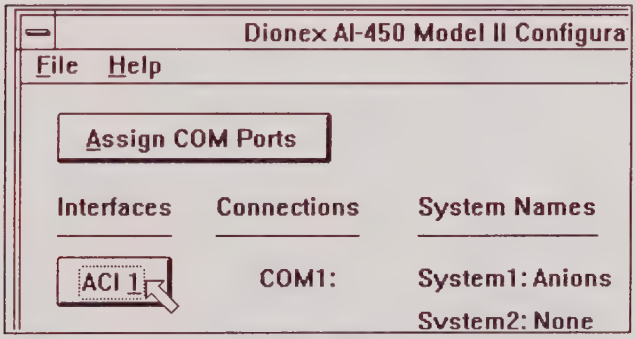


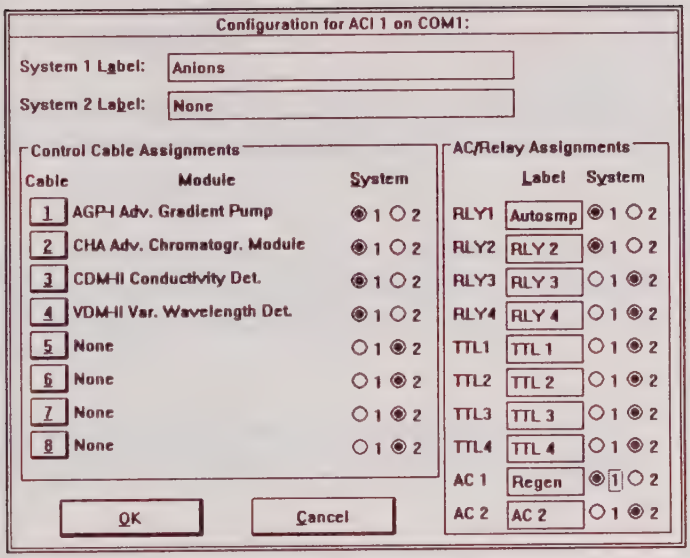


b. Model III



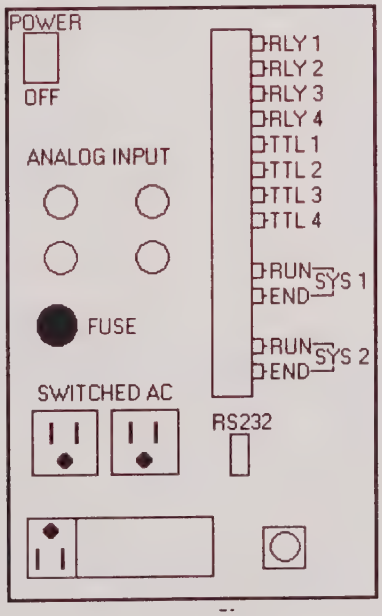
2. Tell the computer how your system is configured





a. Control Cable Assignments are for Dionex Modules with 50-pin Connections
b. Other Devices are controlled by Contact Closure or TTL in the Relay Assignment.
c. AC 1 and AC 2 Control Line Voltage to Devices like Pumps or Coffee Pots.

Back Panel of ACI



EXERCISE 4

A. Click on the Help Menu on MAINMENU and then on the "About MainMenu" command. Which model AI-450 software has been installed on your computer?

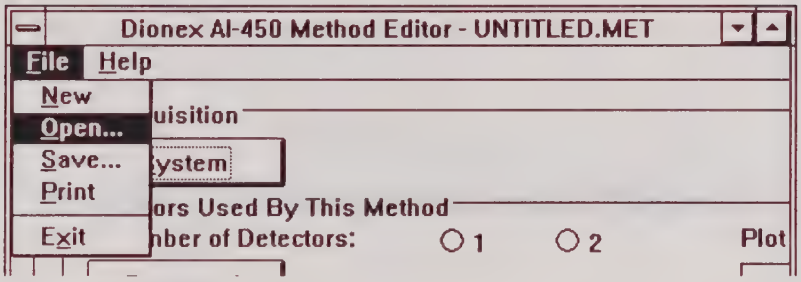
_____

B. Start the CONFIG editor from MAINMENU. Look at the back of the system computer and determine what is connected to the COM ports (these may be labelled as SERIAL ports). Enter this information into the CONFIG editor through ASSIGNing COM PORTS.

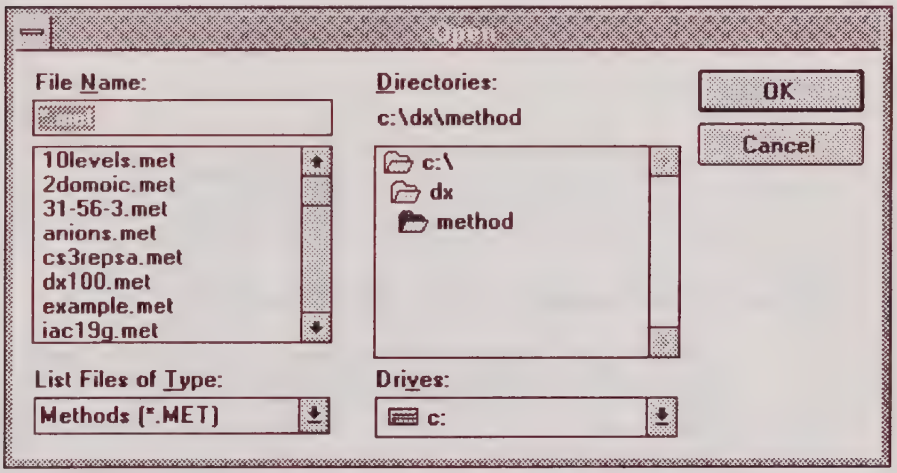
C. Examine the 50-pin ribbon cable connections from the ACI to the Dionex modules and then input this information into the CONFIG editor program.

C. Coordinating Data Collection with METHOD

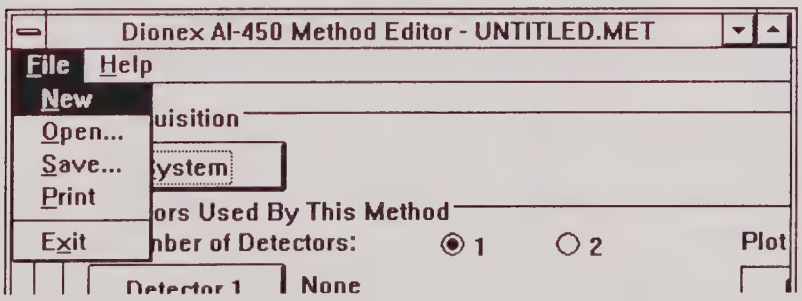
1. Retrieving an Existing Method for Editing



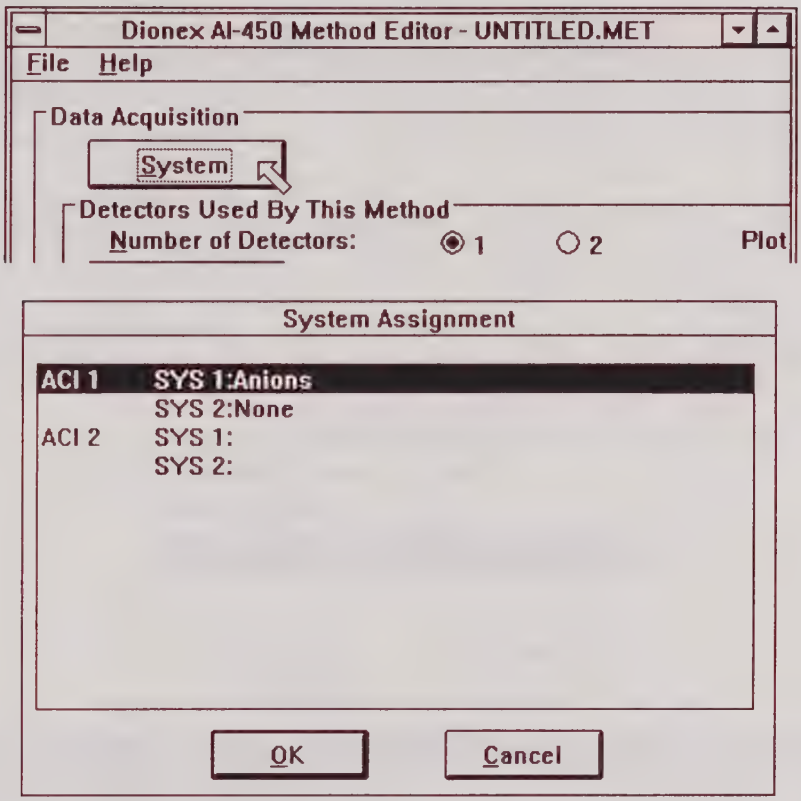
a. Select the Directory and File you wish to retrieve.



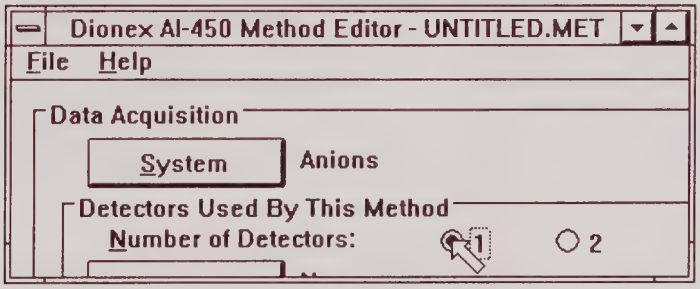
2. Creating a New Method



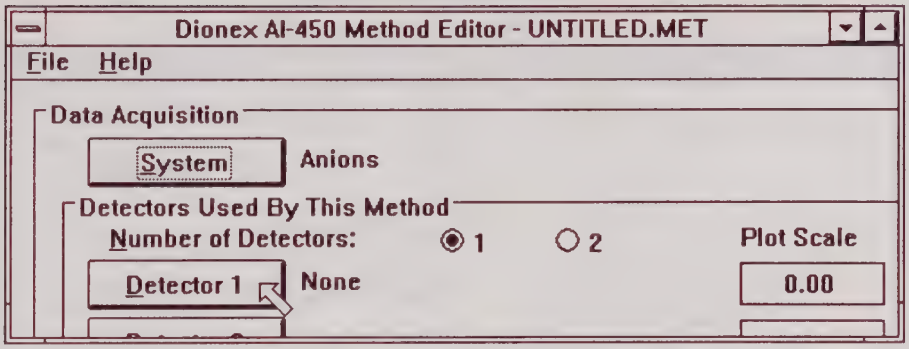
a. Select the System

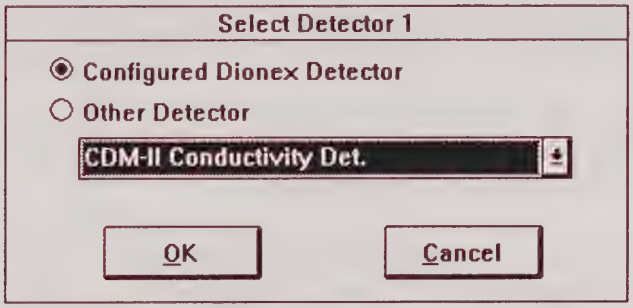


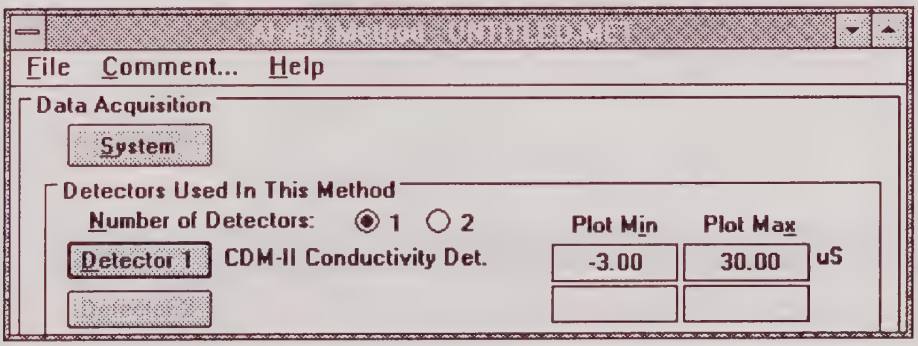
b. Choose the Number of Detectors for this Analysis



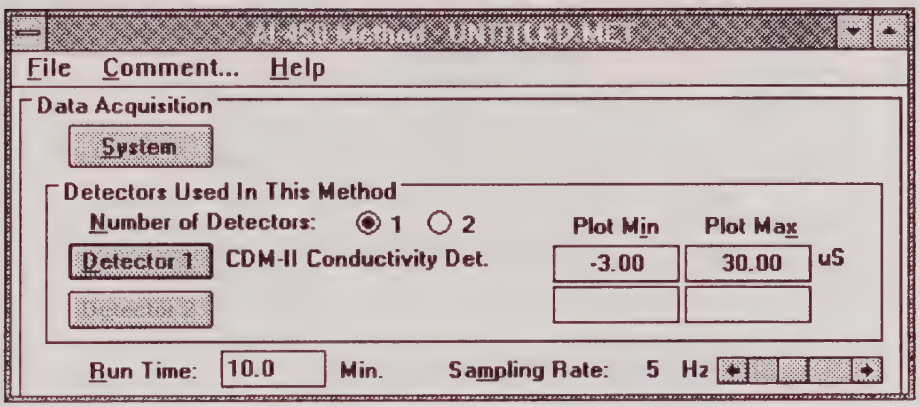
c. Select the Detector(s) to be Used and Set the Plot Scale







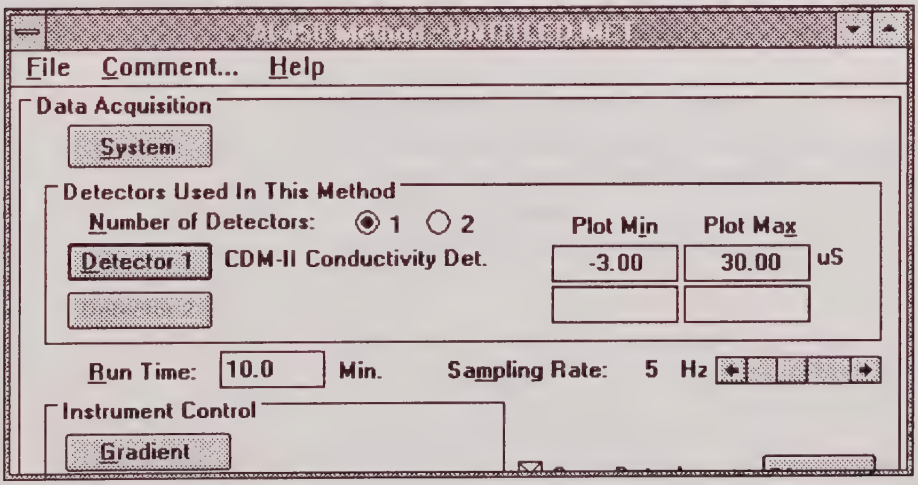
d. Specify the Run-Time (The Actual Amount of Time Data is to be Collected)

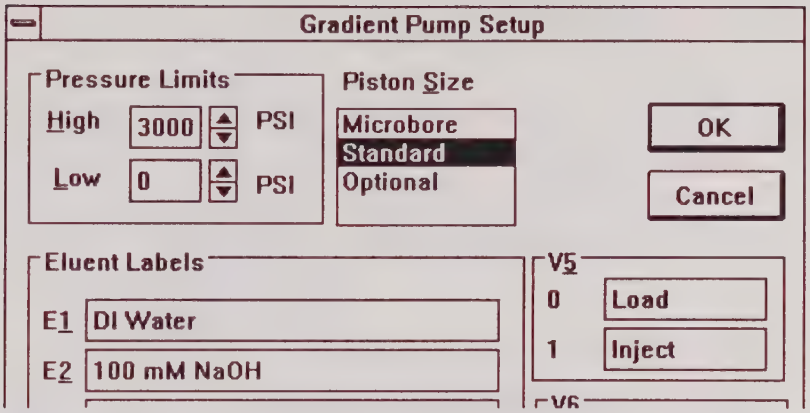


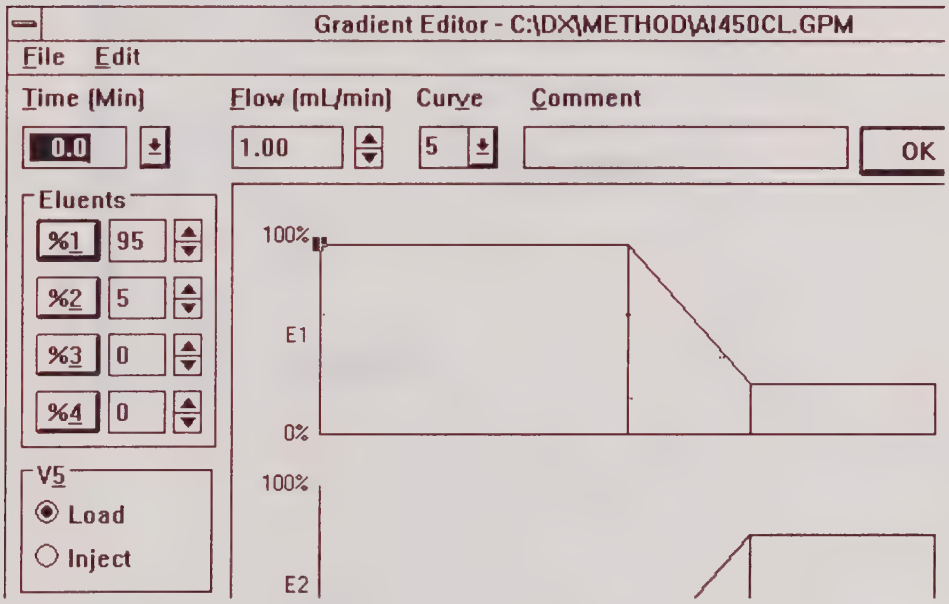
- Run-Time Clock is started by the "Begin Sampling" command in the timed events and stops at the end of the specified Run Time.

e. Specify a **Sampling Rate** (in Hertz [Hz] or data points per second) should be fast enough to collect 50-100 data points across a peak. If it's too fast, the data file for a long run will be very big and take up lots of memory. 5Hz is a good sampling rate for most IC work.

f. Create a Gradient File (if needed)

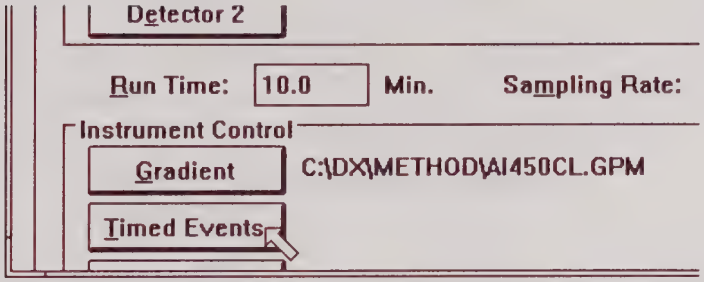


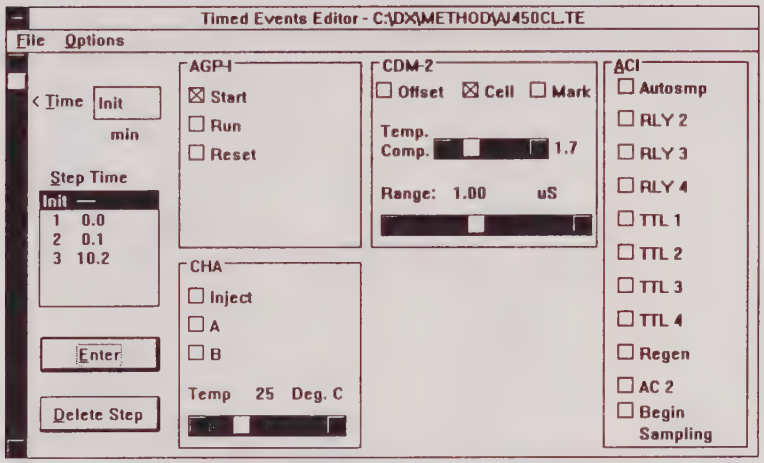




(1) For Systems with GPM or AGP
(2) Gradient Clock is internal to the pump and is controlled in the Timed Events file with Run, Hold, and Reset
(3) Save the .GPM file when finished

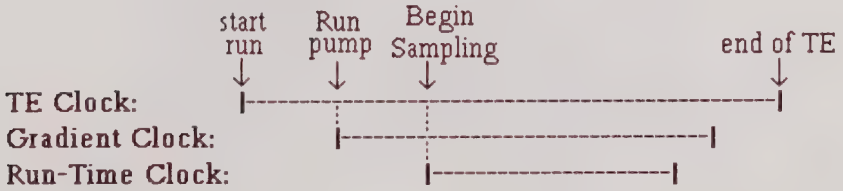
g. Create a Timed-Events (TE) File





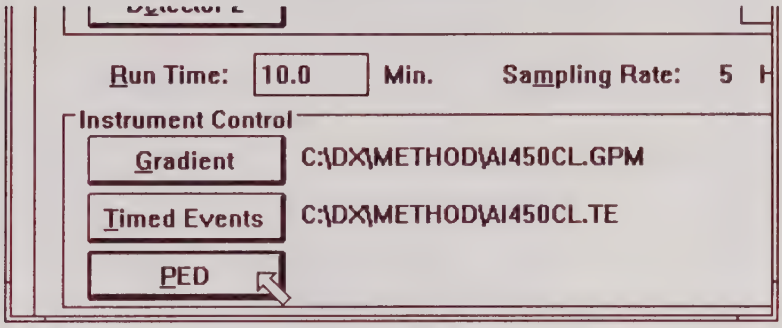
(1) The modules displayed are established in the CONFIG settings.

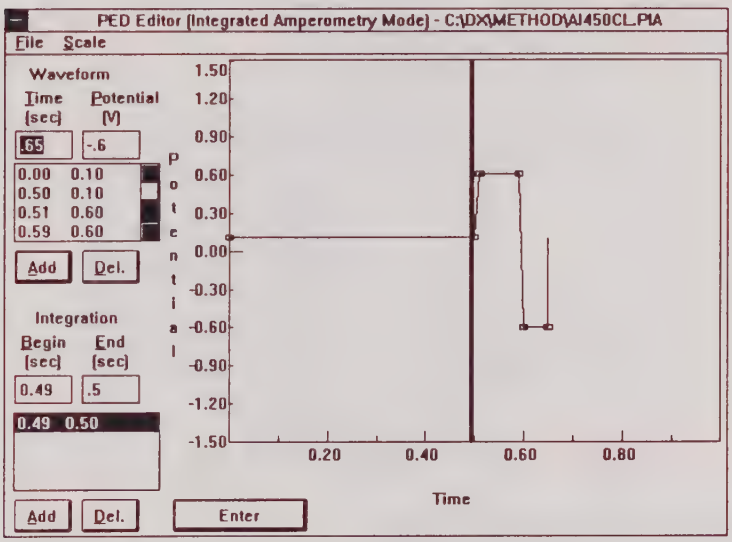
(2) Timed Events Clock is the "master" clock.



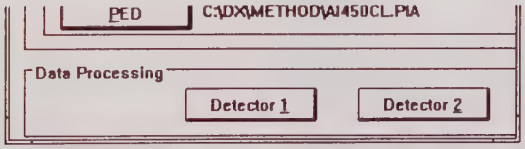
(3) Timed Events are activities (like zeroing your detector) which occur at certain times during the chromatographic analysis. The Timed Events editor is the program used to automate these activities.

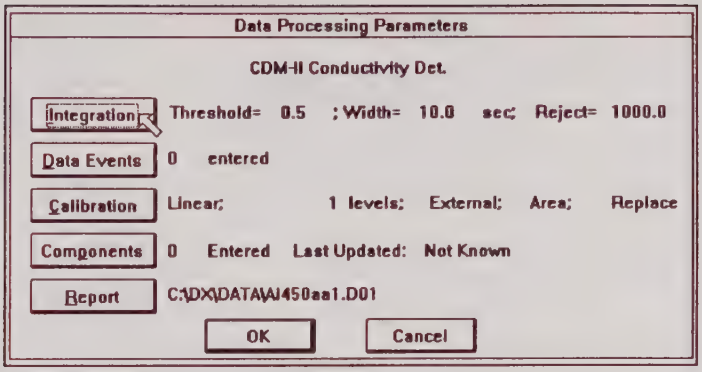
h. PED Programming (Optional for PED users)



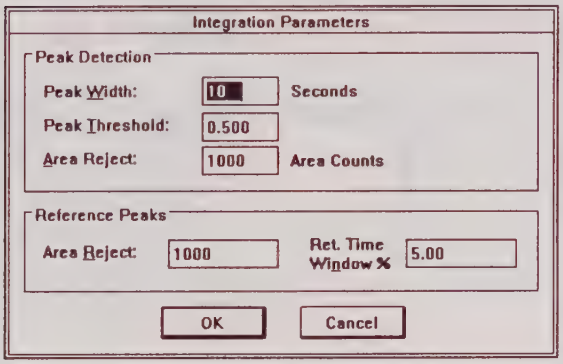


i. Data Processing Parameters





(1) Integration sets the initial integration parameters

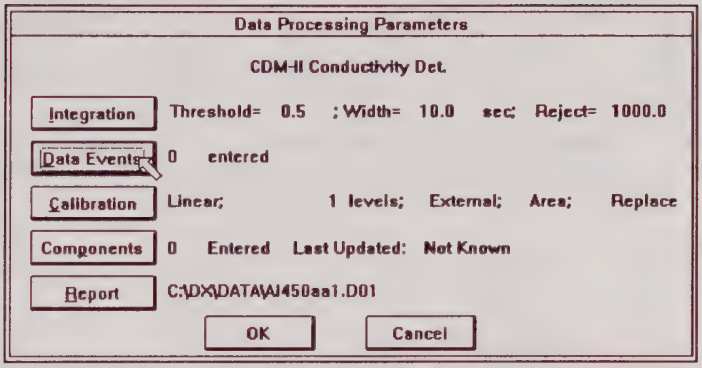


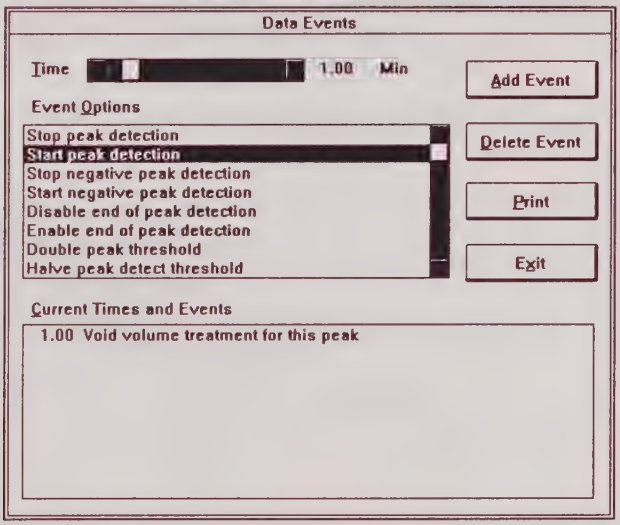
- Peak Width determines the amount of signal filtering or the Bunching Factor. Should be approximately the same as the base width of the first peak in units of seconds.

- Peak Threshold determines the signal level above which a peak is identified. Similiar to noise rejection. Determine with AutoThreshold in OPTIMIZE.

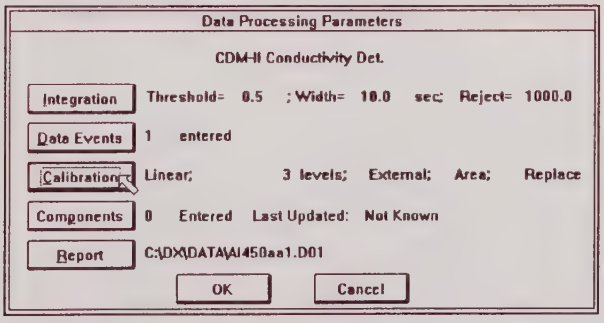
- Area Reject sets the minimum area a peak must have to be reported.

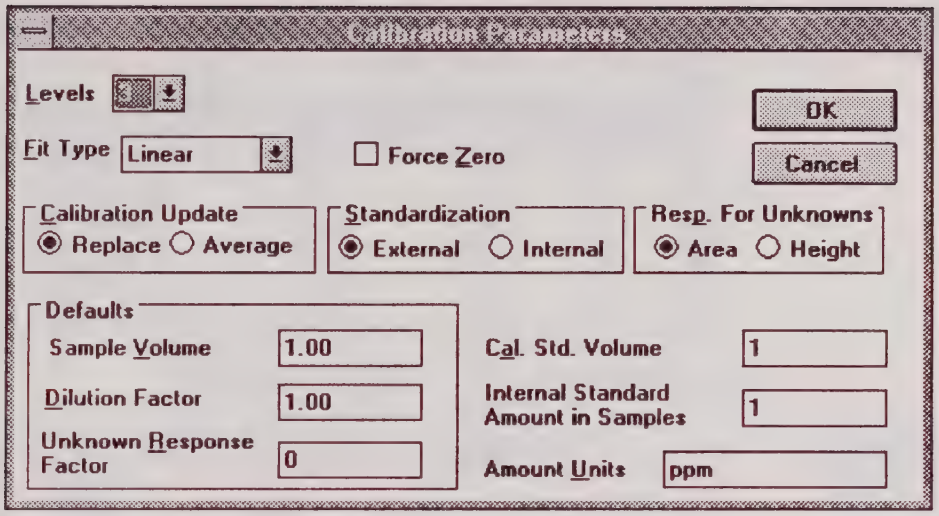
(2) Data Events



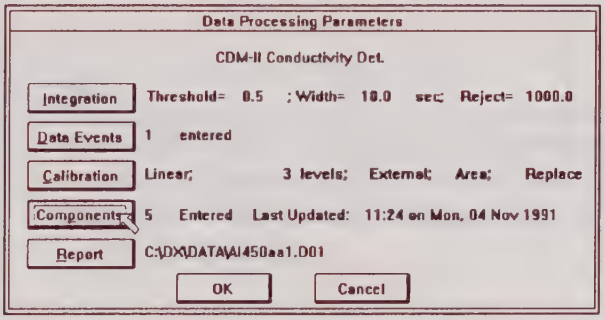


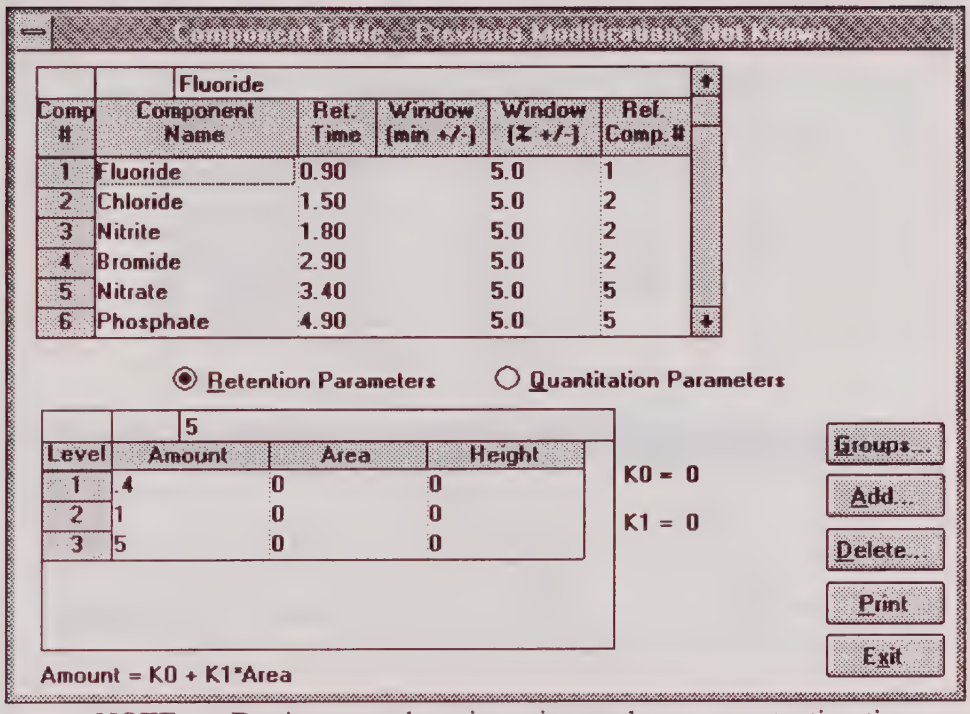
(3) Calibration Parameters





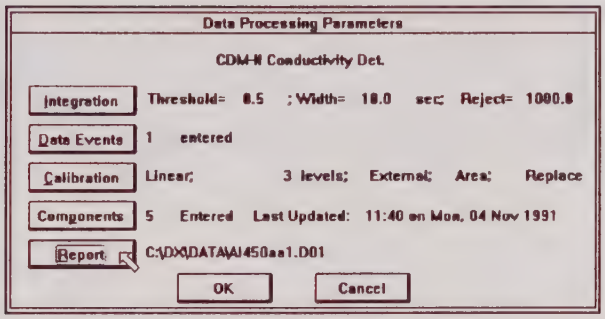
(4) Component Table

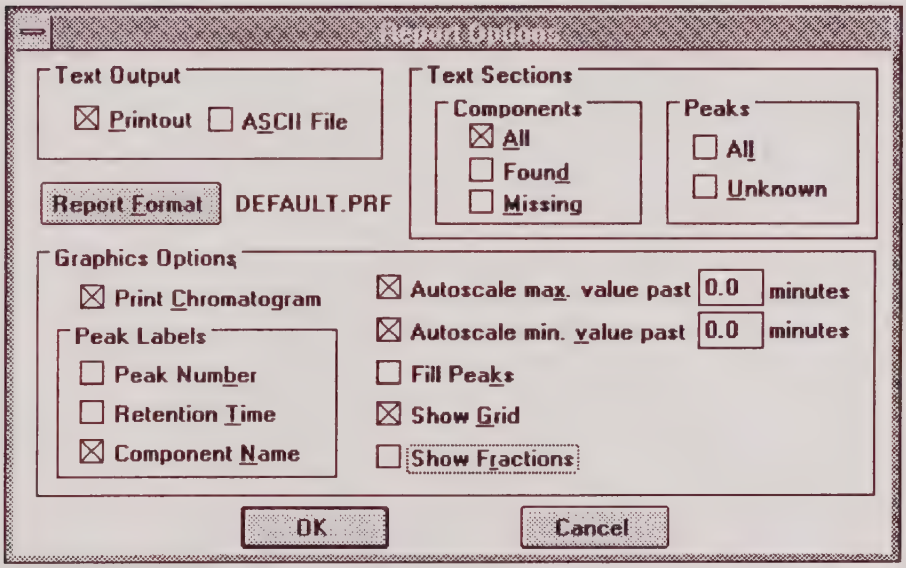



Component Table - Previous Modification: Not Known
Fluoride
Comp # | Component Name | Ret. Time | Window (min +/-) | Window (% +/-) | Ref. Comp. #
1 Fluoride 0.90 5.0 1
2 Chloride 1.50 5.0 2
3 Nitrite 1.80 5.0 2
4 Bromide 2.90 5.0 2
5 Nitrate 3.40 5.0 5
6 Phosphate 4.90 5.0 5
Retention Parameters
Quantitation Parameters
5
Level | Amount | Area | Height
1 .4 0 0
2 1 0 0
3 5 0 0
K0 = 0
K1 = 0
Groups...
Add...
Delete...
Print
Exit
Amount = K0 + K1*Area

NOTE: Don't worry about inputting peak names, retention times, or calibration amounts into the Method before you run the first standard! Methods can be updated after collecting the data using OPTIMIZE.

(5) Report Options



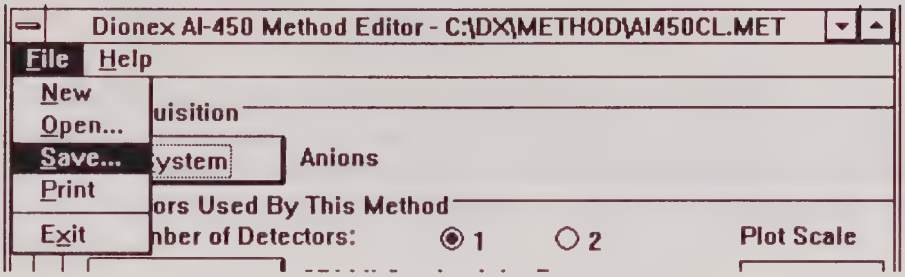


- Data File name is changed by the computer to avoid overwriting old files (the character just to the left of the decimal point is reserved for the detector number - if you're only using one detector, it will always be a "1"):

Method Loaded Once and "Run" Multiple Times:
AI450aa1.D**01**, AI450aa1.D**02**, AI450aa1.D**03**, ...

Method Loaded Over and Over Again (like in a Schedule):
AI450aa1.D01, AI450ab1.D01, AI450ac1.D01, AI450ad1.D01 ....

3. Save the Method when finished.


Dionex AI-450 Method Editor - C:\DX\METHOD\AI450CL.MET
File
Help
New
Open...
Save...
Print
Exit
uisition
ystem
Anions
ors Used By This Method
nber of Detectors:
1
2
Plot Scale

EXERCISE 5

A. You will be running an analysis as described by your instructor. Create a method to operate the Dionex equipment in an automated fashion and collect the data in appropriately-named data files. Details such as system and detector(s) to be used, run time, and components to be analysed will be supplied by your instructor.

B. Save your method under an appropriate name. Print out this method and check it for errors. Ask your instructor for help or advice if needed.

OPTIONAL EXERCISE 5

CREATING A GRADIENT-IC METHOD WITH METHOD

A. Create a method that can be downloaded to the Advanced Computer Interface (ACI) to perform gradient separation of anions on an AG5A-AS5A. The parameters of this system to consider for this method are:

Use the system in the ACI which is configured with a Gradient Pump Module (GPM), an Advanced Chromatography Module (CHA), and a Conductivity Detector Module (CDM-II). You also have an AutoRegen for your regenerant which is plugged into one of the AC outlets on the back of the ACI, and an autosampler which is started by one of the relays on the back of the ACI.

You will only be using only one detector, the CDM-II, to generate the data.

All components and other peaks are eluted in 30 minutes. Because this is typical ion chromatographic analysis, use a sampling rate of 5Hz.

DI water is connected to the Eluent 1 inlet on your GPM, and 100 mM NaOH is connected to the Eluent 2 inlet. The eluent should be pumped through the columns at 1.0 ml/min.

Gradient: Fill out the table on the next page before programming the gradient in the computer. To ensure that all components from the previous run are cleaned off the column, begin your gradient by flushing with 100% Eluent 2 for two minutes and then reequilibrate the column with the initial eluent (5% Eluent 2 and 95% Eluent 1) for ten minutes. Inject your sample and hold the initial conditions for five minutes before ramping to 57% Eluent 2 / 43% Eluent 1 in twenty-five minutes time. Save this gradient program as CLASS.GPM.

Time	% Eluent 1	% Eluent 2	V5	Comment

Timed Events: Fill out the following table before you begin to program the timed events in the computer. You want to INITialize your analysis with the GPM "start"ed, the CDM cell ON, and your AutoRegen unit ON. The autosampler module takes about 2.5 minutes to run through its loading process for each sample. This sample loading can be done while the column is being reequilibrated to the initial conditions. The relay control for the autosampler only needs to be turn on momentarily to start the autosampler, so you can turn the relay off 0.1 minutes after you start it. Remember to "Begin Sampling" at the same time you switch the injection valve from LOAD to INJECT from the CHA or when V5 is turned on in the gradient program. After the run time is complete, HOLD (that is "NOT" RUN) the gradient program and RESET the GPM. Save this timed events file as CLASS.TE.

Time	Event Description	Status
Init		

Data Processing Parameters: The **Integration, Data Events, Calibration Table,** and **Component Table** parameter entry are optional (see next page). These parameters can all be entered post-run through the OPTIMIZE program.

Report Options: You will want to print a report and processed plot when the run is complete and the plot should be autoscaled to keep all the peaks on scale. The raw data can be saved in data files starting with the name:

C:\DX\DATA\GRDANION\ANIONAA1.D01.

---------- Optional ----------

Integration Parameters: Start with a Peak Width of 3 seconds and a Peak Threshold of 0.5. Set the Area Reject to report peaks with areas greater than 1000 counts.

Data Events: To avoid detecting noise before the water dip, Stop Peak Detection at the beginning of the Run Time and Start Peak Detection just before the fluoride peak elutes (about 2.2 minutes).

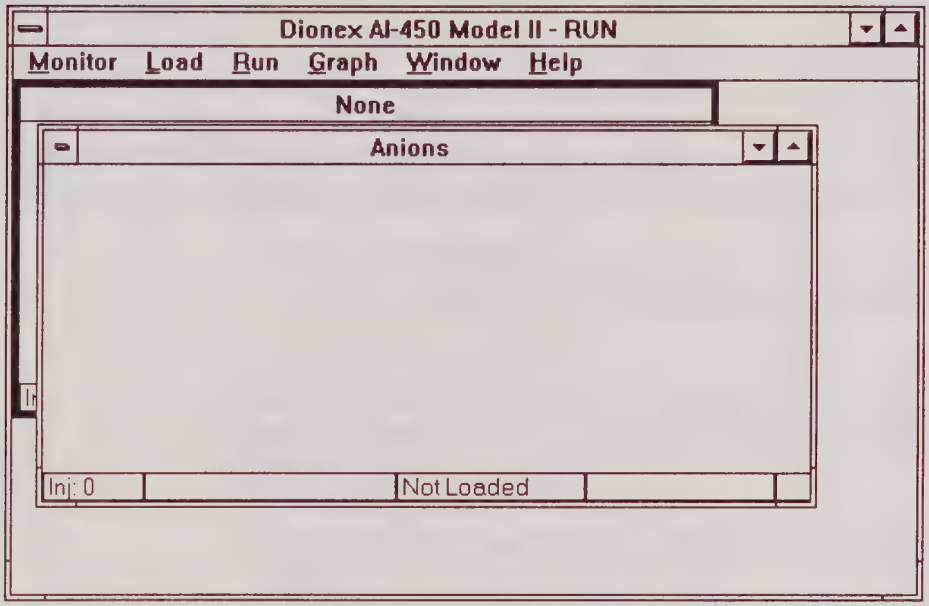
Calibration Table: You will be running a three-level external standard calibration which should be linear and will be replacing previous calibration values with new peak areas. The units of concentration are parts-per-million.

Component Table: The three components you will be analyzing are Fluoride (retention time 2.9 min), Chloride (RT=11.1 min), and Sulfate (RT=16.8 min). Make sure they reference themselves to prevent misidentification of peaks.

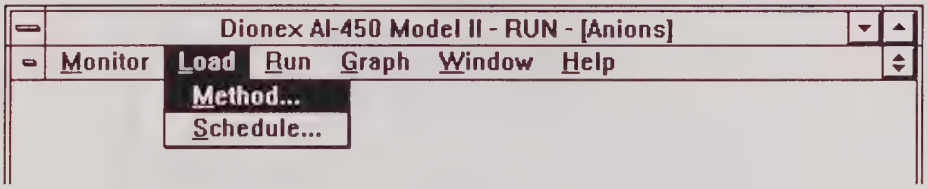
B. Save this method as "C:\DX\METHOD\CLASS.MET and print the method out.

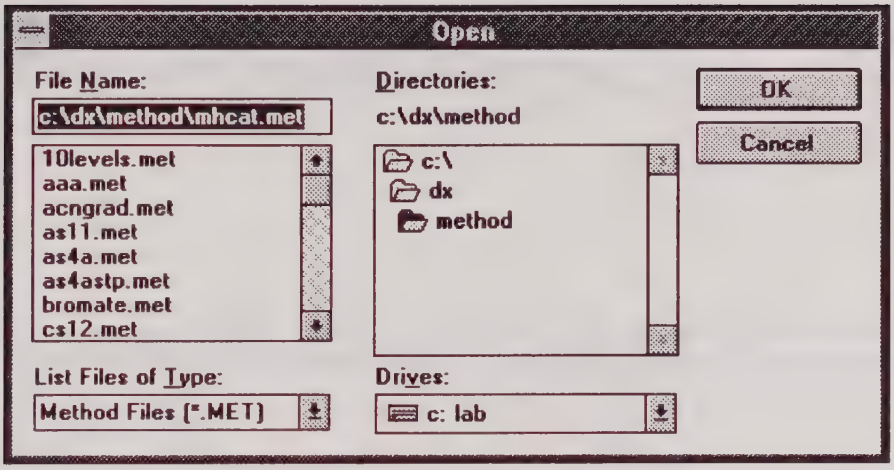
D. Collecting Data with RUN

1. Initial Screen shows multiple Windows (one Window for every system) - if using only one system, close other Windows.



2. Load a Method or a Schedule (we will cover Schedule loading after discussion of Schedules) into the System ACI

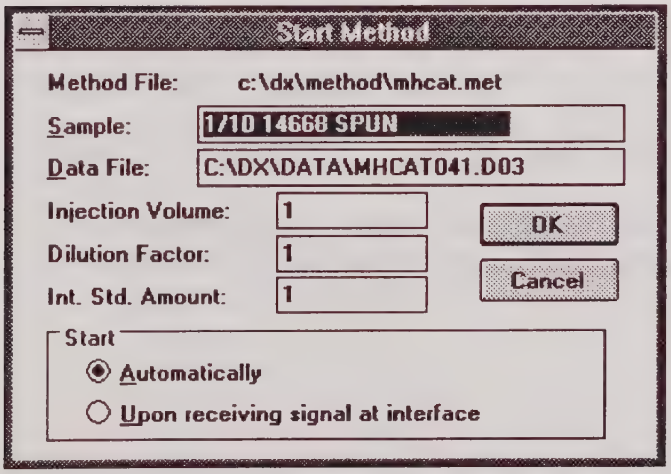


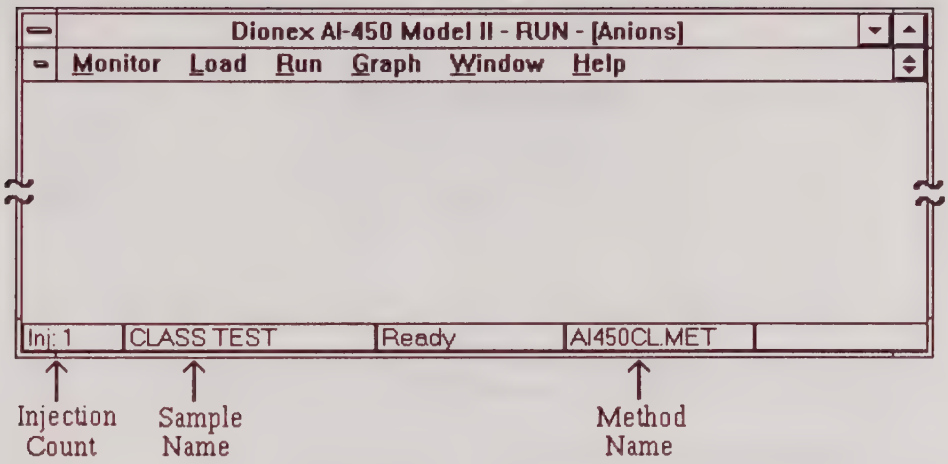


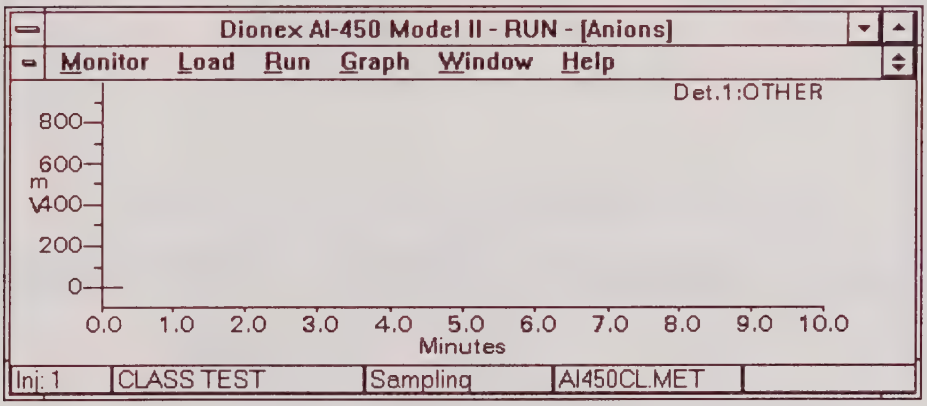
-Click the OK Button.
-Note the method loads but no sample name is loaded.

3. To start the Timed Events clock, click on RUN and START to recieve a text box in which you indicate the sample name and file name.

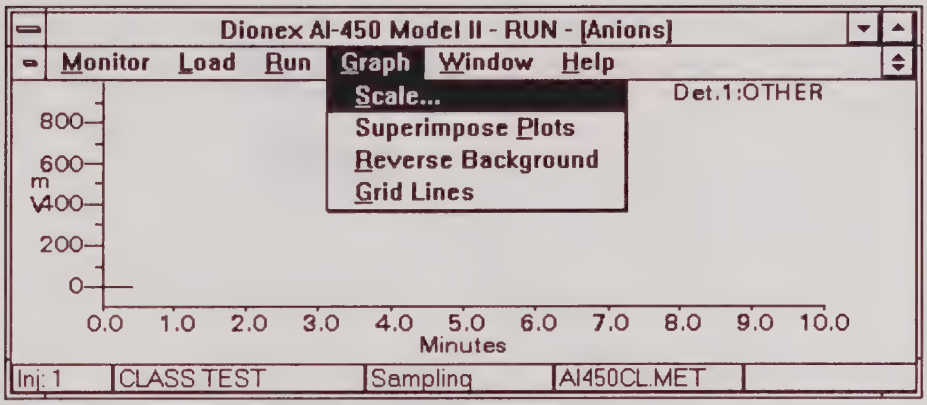
-Click on run automatically or upon recieving a signal at ACI.
-Click on OK button.



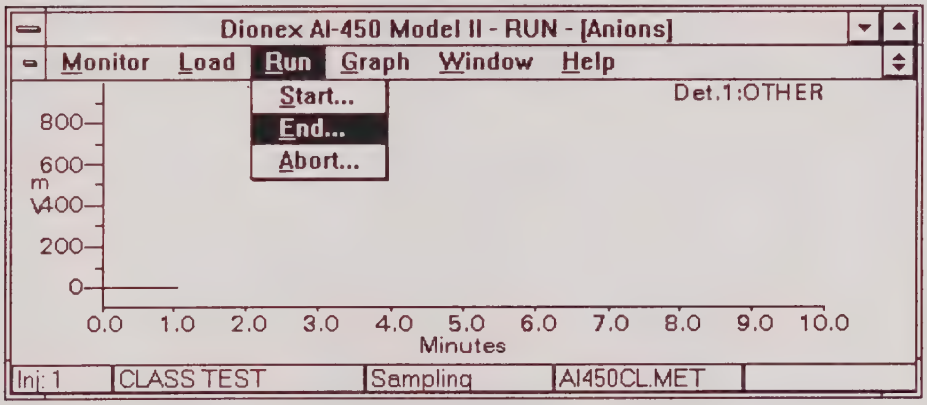


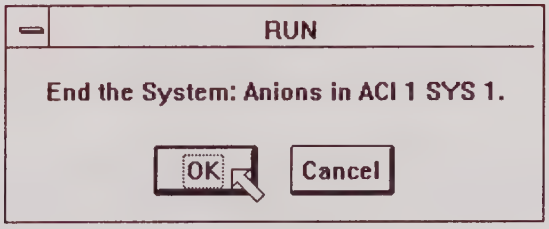


4. Change the Scale or other Screen Parameters using the commands in the GRAPH menu. These changes are NOT reflected in the printout.

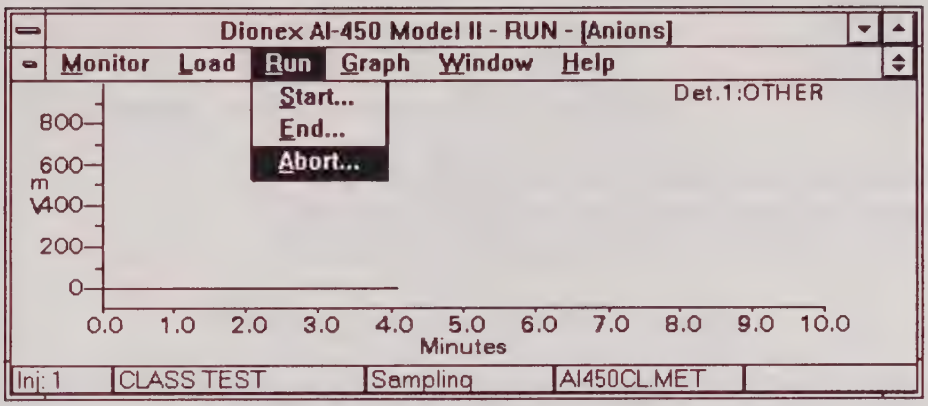


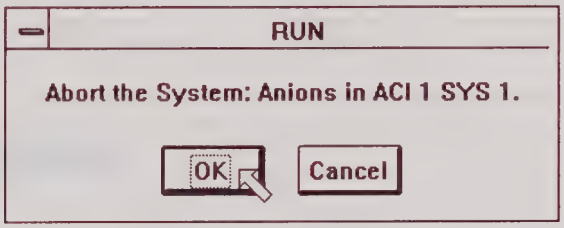
5. End Data Collection and Process the Data Taken So Far by Pressing the Yellow END Button on the ACI or Selecting the END command from the Run Menu.





6. Abort the Data Collection and Throw Out the Data Collected So Far by Pressing the Red ABORT Button on the Front of the ACI or by Selecting the Abort Command in the Run Menu. (Note: when aborting a run no information is saved and no report is generated.)





EXERCISE 6

A. Check the chromatographic system you have been provided to see that it is stable and ready for an injection (ask the instructor for help if necessary).

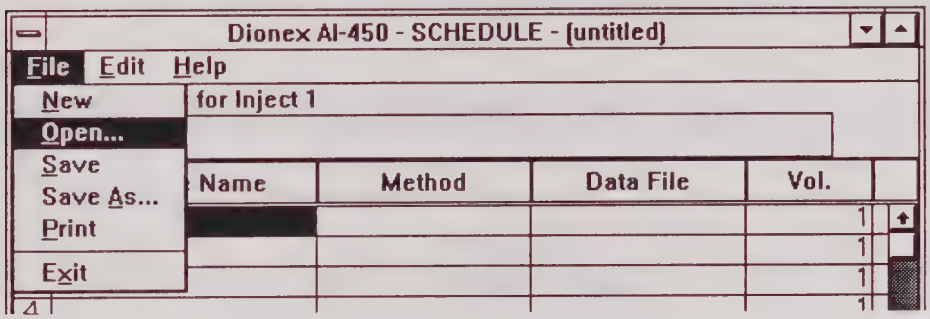
B. Start the RUN program, and load the Method you created in Exercise 5 into the Advanced Computer Interface (**NOTE:** If you are collecting data with a different computer than the one on which you created your method, you will **FIRST** need to copy your method files onto a floppy disk, and then copy these files from the floppy disk into the METHOD subdirectory on the system computer. Ask your instructor for help if you are unsure of how to do this). Load your sample or standard into the injection valve and push the green RUN button on the ACI to begin the timed events and data collection.

C. When the run is finished, the data stored, and the report printed out (if any), use the File Manager program to see if the data file was stored in the proper subdirectory.

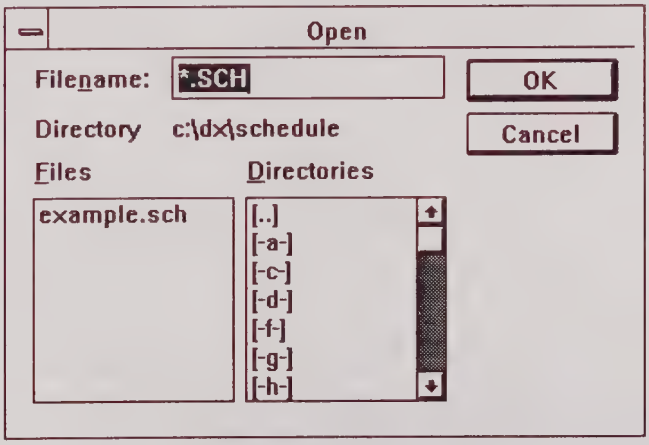
E. Running Multiple Samples Using SCHEDULE

- using SCHEDULE to collect data from multiple samples allows the use of different sample names and different methods for each injection.

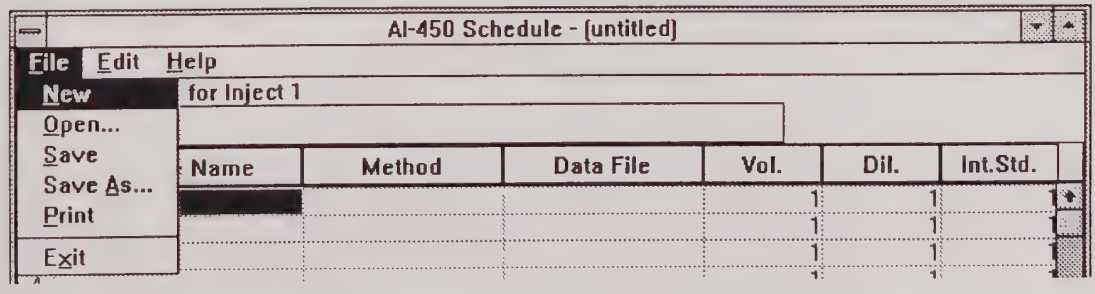
1. Retrieving an Existing Schedule for Editing.



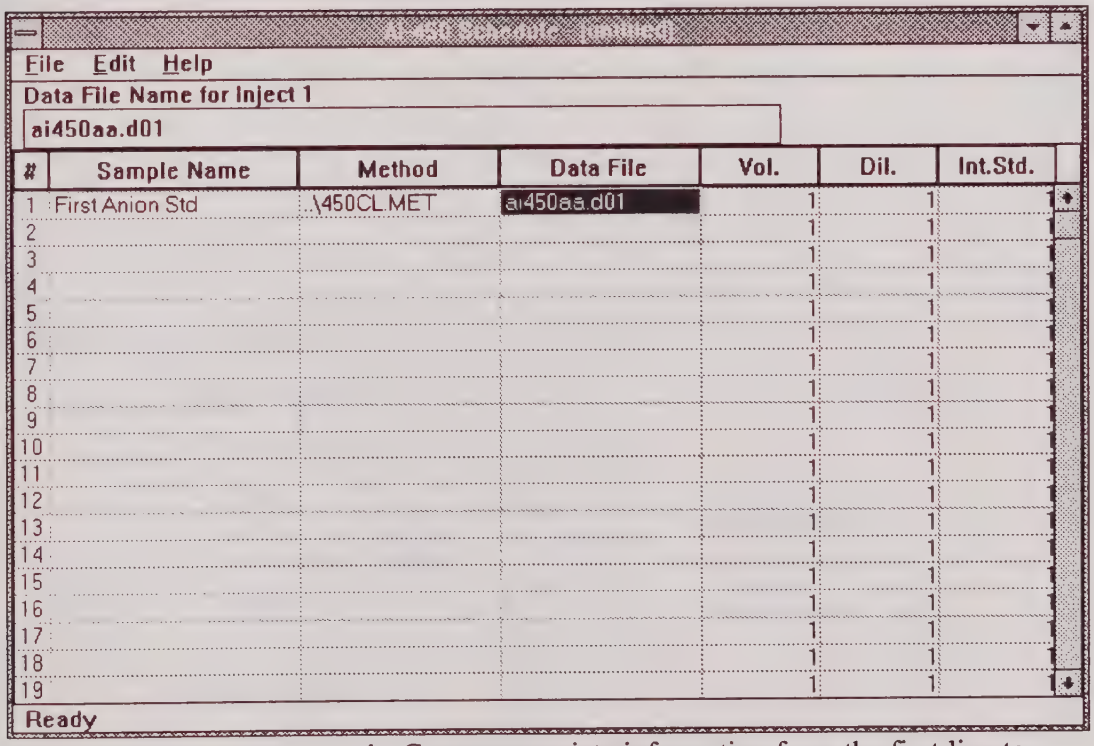
a. Select the Directory and File you wish to retrieve.



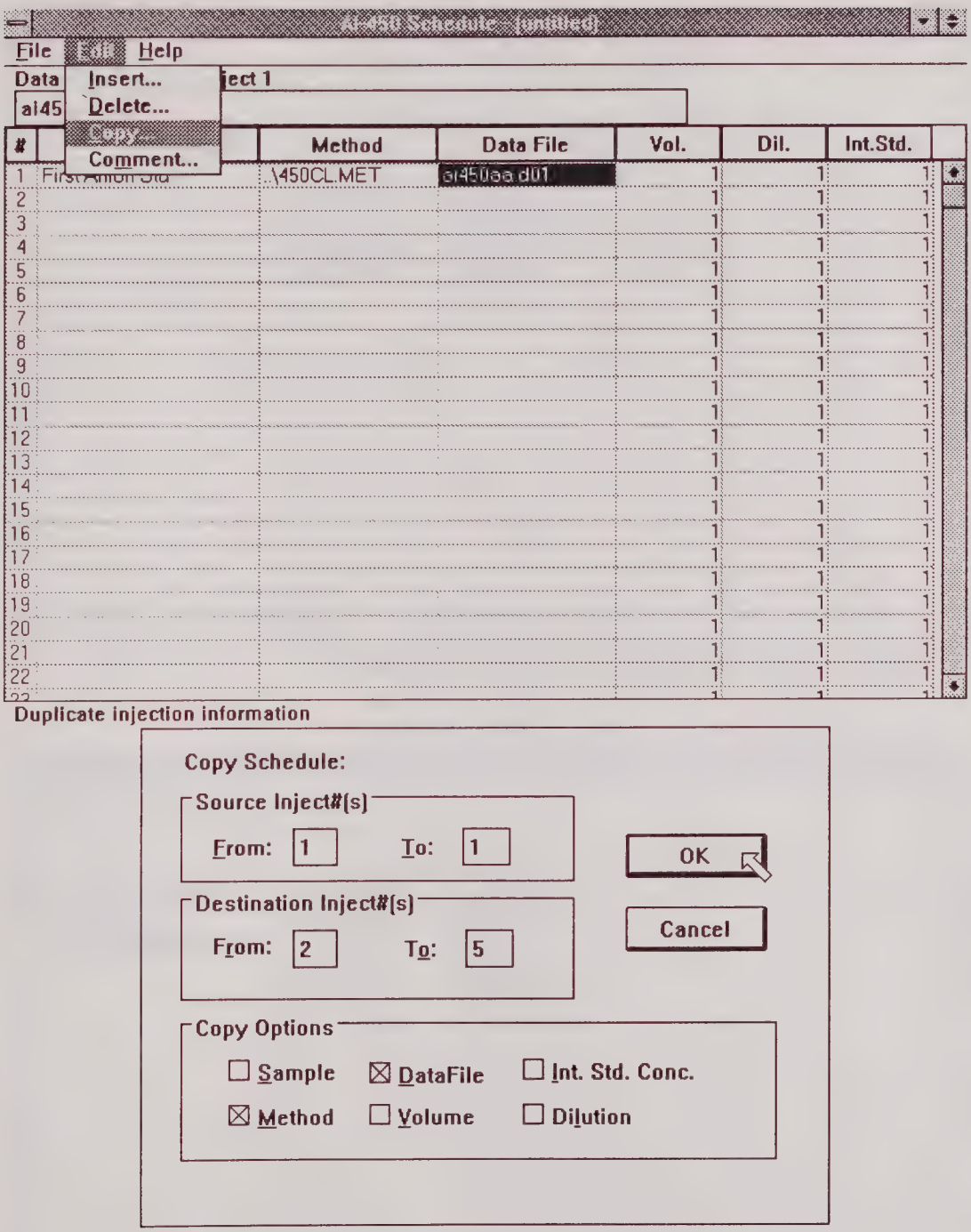
2. Creating a New Schedule

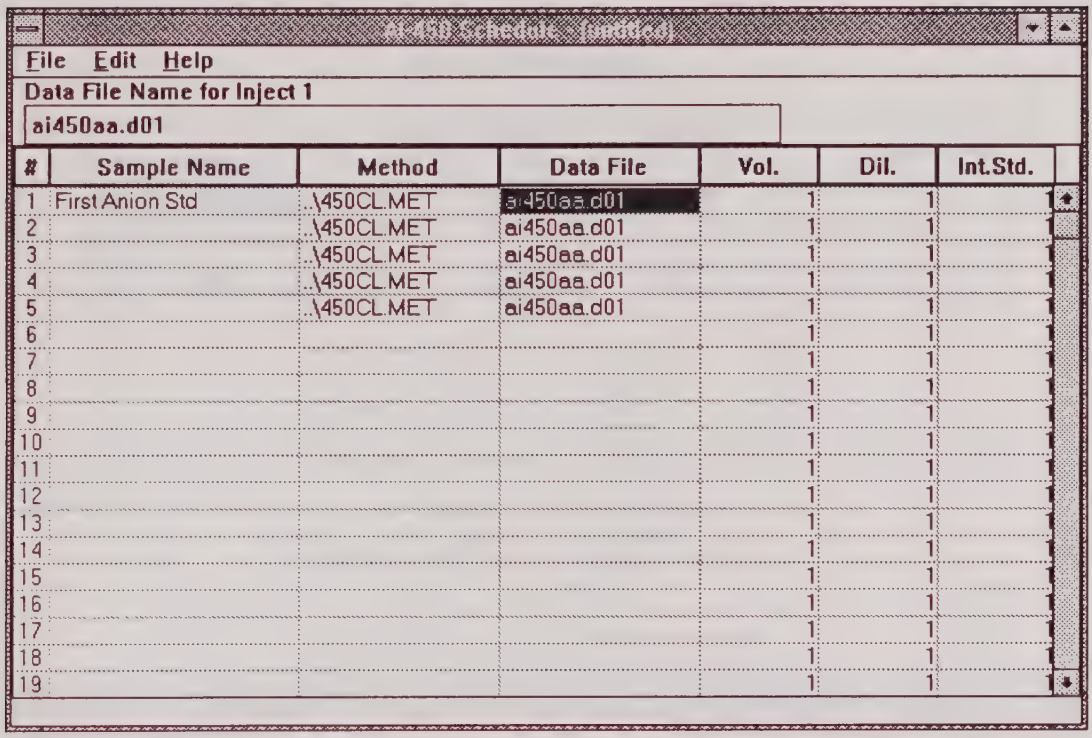


a. Enter the Sample Name, Method, and Data File for First Sample.
   -Click on method field to display methods on disk.
   -Date file names do not need path because the path is indicated in the RUN program when loading the schedule.



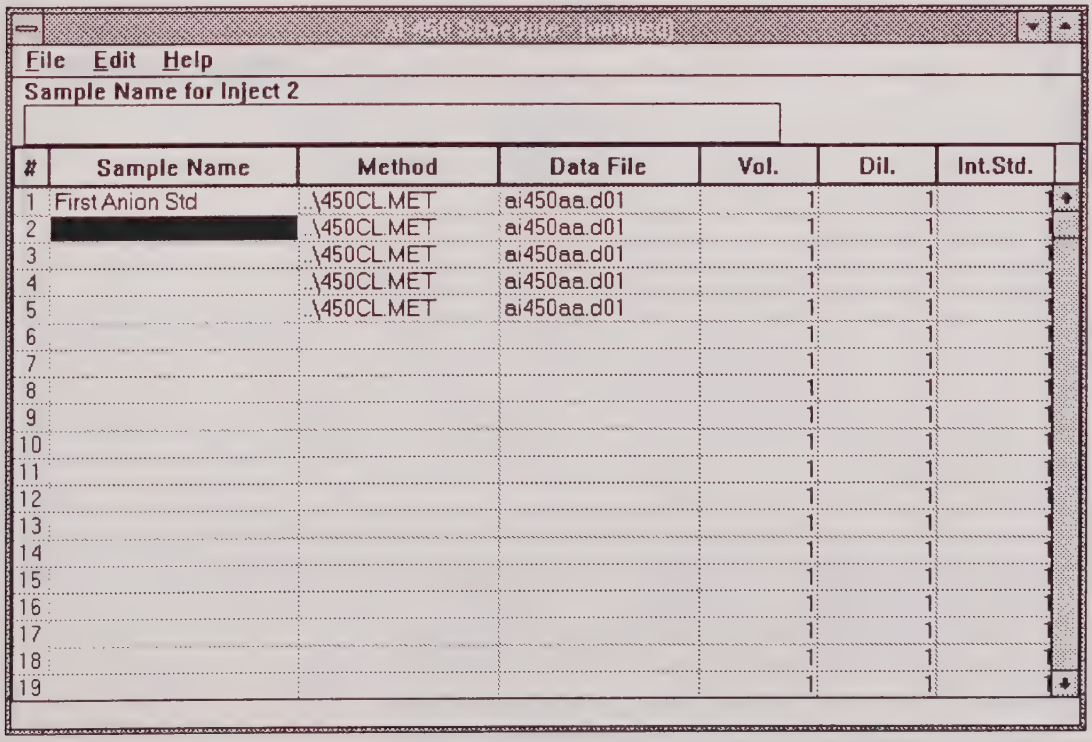
b. Copy appropriate information from the first line to subsequent lines (**NOTE:** Be sure to "un-X" any Option you don't want copied or the copy function will write over changes you've made).


AI-450 Schedule - [untitled]
File
Edit
Help
Data
Insert...
Delete...
Copy...
Comment...
ai45
ject 1
#
Method
Data File
Vol.
Dil.
Int.Std.
1
First Anon Std
.\450CL.MET
ai450aa.d01
Duplicate injection information
Copy Schedule:
Source Inject#(s)
From:
1
To:
1
Destination Inject#(s)
From:
2
To:
5
OK
Cancel
Copy Options
Sample
DataFile
Int. Std. Conc.
Method
Volume
Dilution



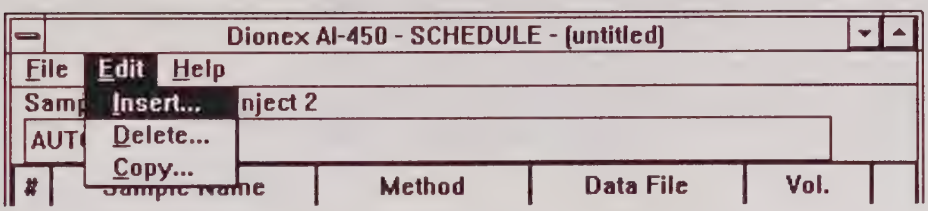
#	Sample Name	Method	Data File	Vol.	Dil.	Int.Std.
1	First Anion Std	.\450CL.MET	ai450aa.d01	1	1	
2		.\450CL.MET	ai450aa.d01	1	1	
3		.\450CL.MET	ai450aa.d01	1	1	
4		.\450CL.MET	ai450aa.d01	1	1	
5		.\450CL.MET	ai450aa.d01	1	1	
6				1	1	
7				1	1	
8				1	1	
9				1	1	
10				1	1	
11				1	1	
12				1	1	
13				1	1	
14				1	1	
15				1	1	
16				1	1	
17				1	1	
18				1	1	
19				1	1	

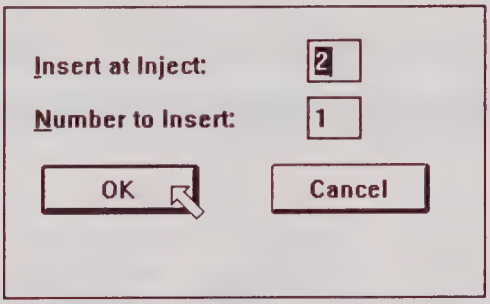
c. Edit Each Line by Clicking on the Cell to be Edited and then Making the Change in the Edit Box

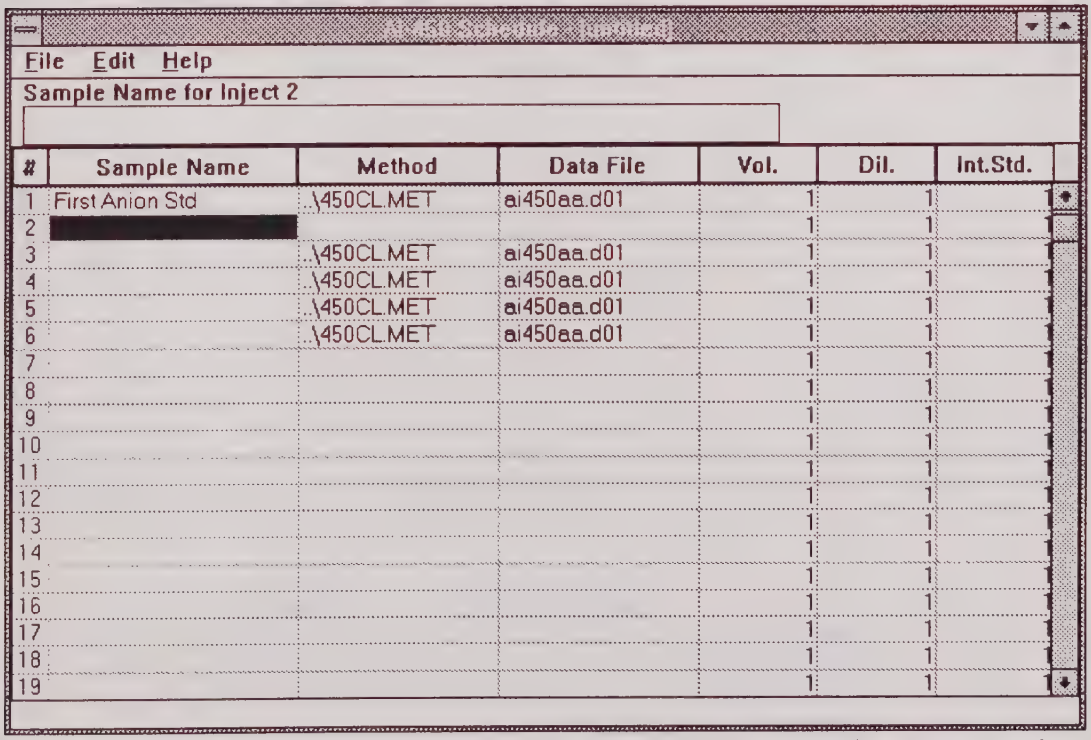


#	Sample Name	Method	Data File	Vol.	Dil.	Int.Std.
1	First Anion Std	.\450CL.MET	ai450aa.d01	1	1	
2		.\450CL.MET	ai450aa.d01	1	1	
3		.\450CL.MET	ai450aa.d01	1	1	
4		.\450CL.MET	ai450aa.d01	1	1	
5		.\450CL.MET	ai450aa.d01	1	1	
6				1	1	
7				1	1	
8				1	1	
9				1	1	
10				1	1	
11				1	1	
12				1	1	
13				1	1	
14				1	1	
15				1	1	
16				1	1	
17				1	1	
18				1	1	
19				1	1	

d. Insert a Blank Line When a New Sample Needs to be Added in the Middle.





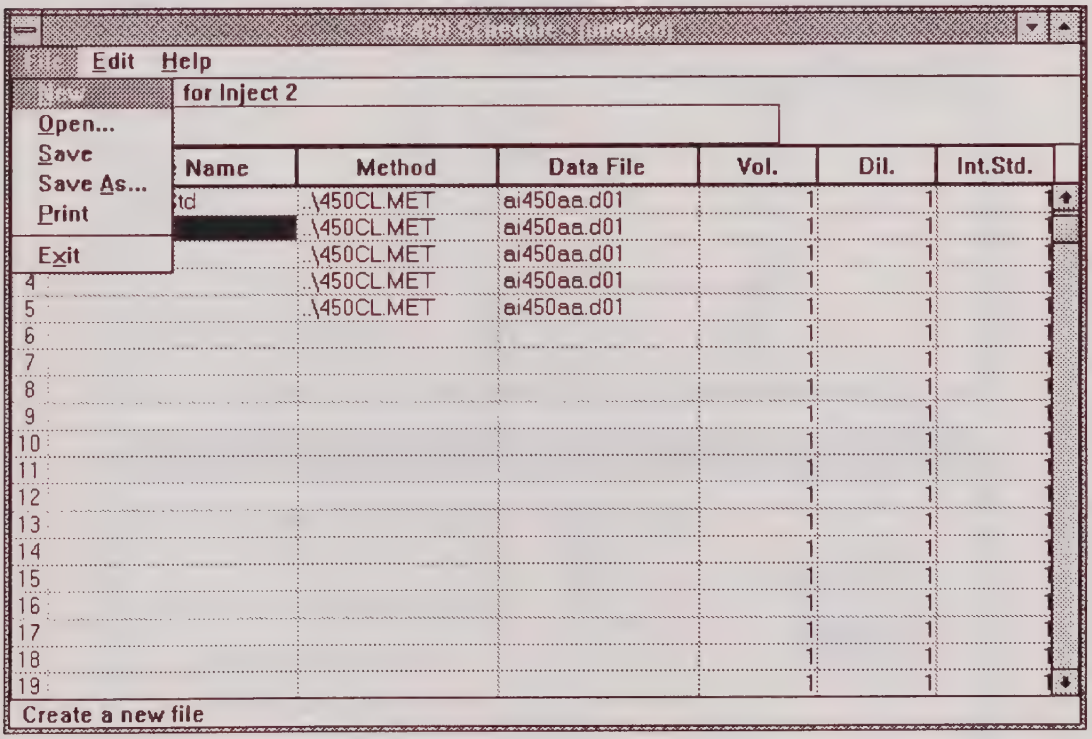


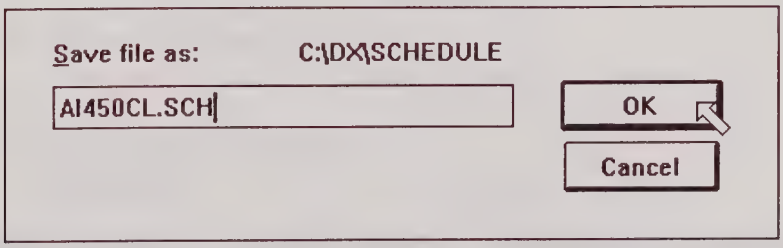
#	Sample Name	Method	Data File	Vol.	Dil.	Int.Std.
1	First Anion Std	..\450CL.MET	ai450aa.d01	1	1	1
2				1	1	1
3		..\450CL.MET	ai450aa.d01	1	1	1
4		..\450CL.MET	ai450aa.d01	1	1	1
5		..\450CL.MET	ai450aa.d01	1	1	1
6		..\450CL.MET	ai450aa.d01	1	1	1
7				1	1	1
8				1	1	1
9				1	1	1
10				1	1	1
11				1	1	1
12				1	1	1
13				1	1	1
14				1	1	1
15				1	1	1
16				1	1	1
17				1	1	1
18				1	1	1
19				1	1	1

e. "AUTOCALnA" or "AUTOCALnR" are Key Words in a Schedule and Indicate that the Sample Being Injected is a Calibration Standard (**n** indicates the level of the standard; e.g. AUTOCAL1R or AUTOCAL1A for the lowest level standard) and the Area and Height

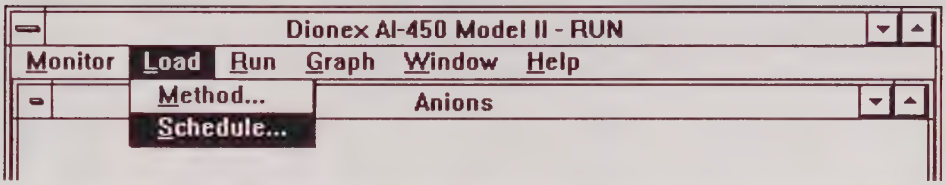
from the Run Should be Transferred to the Appropriate Level in the Method. The "A" or "R" at the End Indicates Whether the Responses from this Calibration Run Should be Averaged with the Previous Responses in the Method or Replace the Previous Responses. (The A or R are not required if no change is being made from what is in the method.)

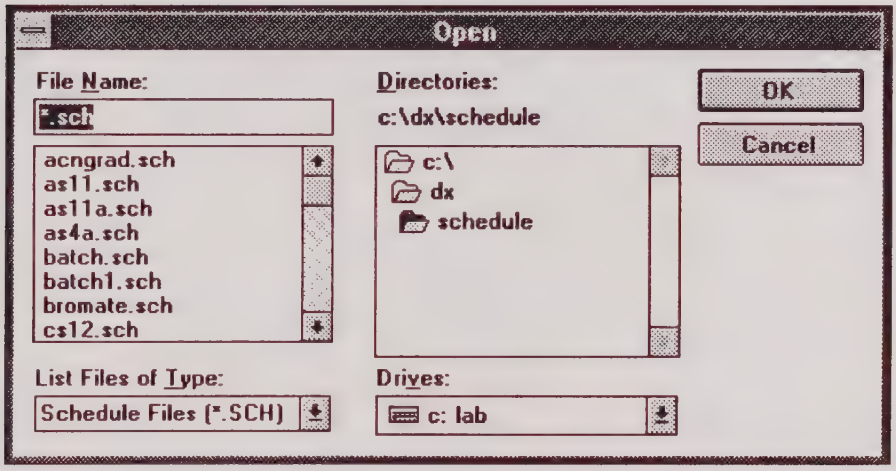
3. Save the Schedule When Editing is Complete

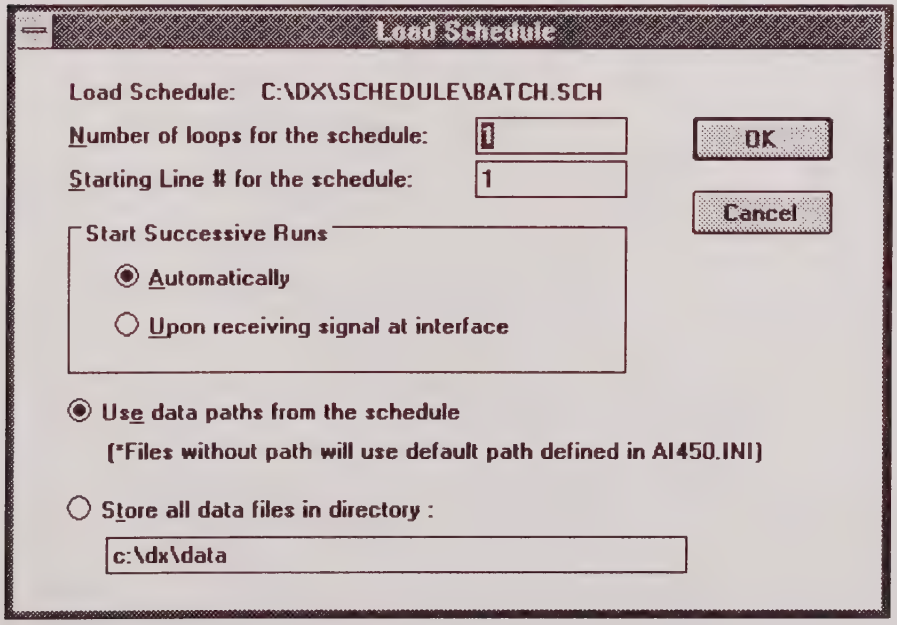




4. Loading a Schedule into RUN







- If an autosampler is used, successive runs can be automatically by the computer and all samples analysed unattended. If each sample is loaded manually into the injection valve, a schedule can still be used to let the

computer automatically load the next sample name and method. Once the next sample is loaded, the operator needs only to push the green RUN button on the ACI to start the next run. The next method in the schedule is loaded into the ACI at the end of each run.

EXERCISE 7

CREATING A SCHEDULE OF IC RUNS

A. You will be using SCHEDULE to collect data from three calibration standards and a couple of samples. Create a schedule based on what your instructor tells you the standards and samples are. Use the copy command as much as possible.

On all runs
Method = Method you created in Exercise 3 for data collection.
Data file = Data file specified in the above Method (the names can initially all be the same - the computer will change their names on the disk and in the schedule to prevent overwriting)
Volume = 50
Dilution = 1

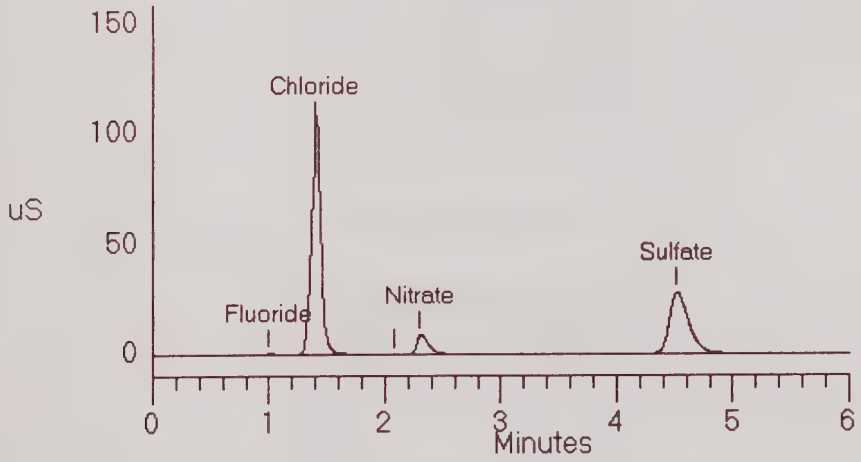
B. Save this schedule as C:\DX\SCHEDULE\CLASS.SCH

C. Print this schedule

```
==========================================================
| Sample Name: SAN JOSE TAP WATER NO DILUTION Date: Tue Jul 24 15:27:41 1990 |
| Data File  : C:\DX\DATA\AI450SJW.D01                                       |
| Method     : C:\DX\METHOD\AI450CL.MET                                      |
| ACI Address: 1      System : 1      Inject#:  1  Detector: CDM-1           |
==========================================================
```

REPORT	VOLUME	DILUTION	POINTS	RATE	START	STOP	AREA REJ
External	1	1	1805	5Hz	0.00	6.02	1000

Pk. Num	Ret Time	Component Name	Concentration ppm	Height	Area	Bl. Code	%Delta
1	1.02	Fluoride	1673.600	323	1674	1	-0.33
2	1.40	Chloride	593309.600	103685	593310	1	0.00
3	2.30	Nitrate	60991.300	8518	60991	1	0.00
4	4.52	Sulfate	319531.000	27870	319531	1	-0.07
		Totals	975505.500	140396	975506		



A. What information is in the report?

1. HEADER INFORMATION
   a. Sample Name: The name given at the time data was collected.
   b. Date: Date the data was collected
   c. Data File: File where data and method information is stored.
   d. Method: Last method used to integrate the data.
   e. System Information: The ACI address, System number, Injection number and Detector used to collect the data.

2. REPORT BODY
    a. Report: Type of report, e.g. external standard
    b. Volume and Dilution: Factors included in Method or Schedule for scaling purposes.
    c. Points: Number of data points in the data file (which is the Sampling Rate times the number of seconds of the run - e.g. 5Hz * 6.02 min * 60 sec/min = 1806 points)
    d. Rate: Sampling rate for the run
    e. Start and Stop: The start and stop times for the chromatographic plot
    f. Area Rej: The area rejection value used for the integration
    g. Columns of the Report depend on the Report Format (as specified in the Report section of the Data Processing Options in the method). Most are self explanatory, but the following need definition:

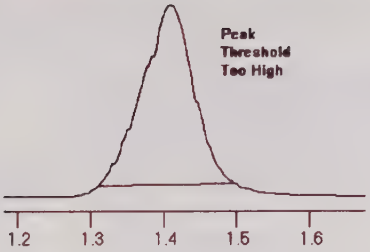
        Bl. Code: Baseline Code explains how the peak was integrated. BL =1 means completely resolved peaks, BL=2 indicates partially resolved peaks of similar height, BL=3 means the peak is a "mother" peak with other peaks on the shoulder(s), and BL=4 indicates the shoulder peaks.

        %Delta: The percent deviation in retention time for the found peak retention time from the expected retention time in the method.

B. Remedies for Ailing Chromatograms using METHOD

1. Peaks should be properly named. If the peaks are misidentified or not identified, this indicates either that there's a problem in the chromatography or that the Retention Time or % Time Window information in the method needs to be updated.

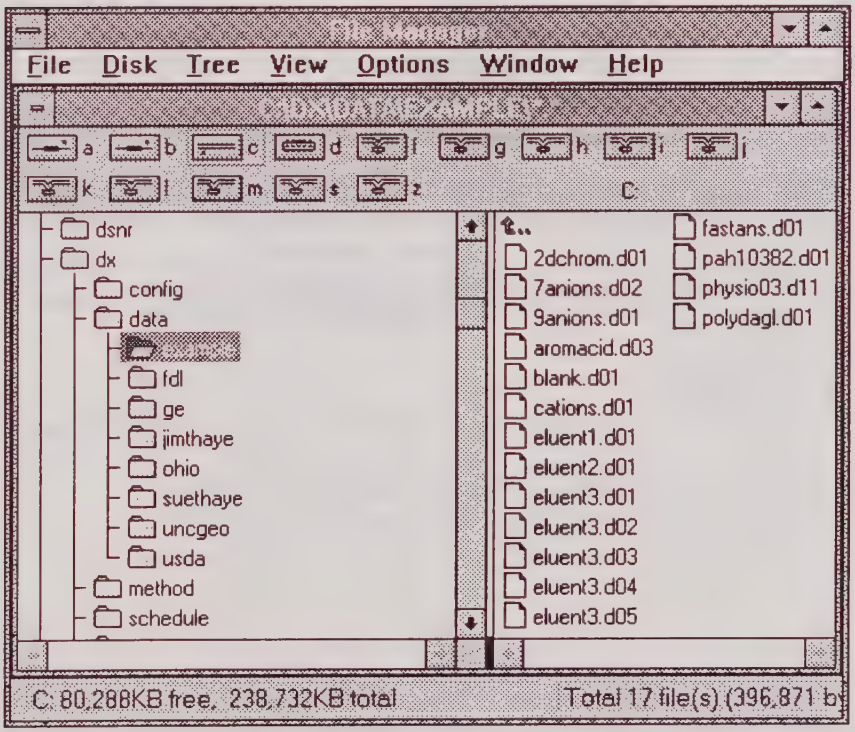
2. Peaks should be properly integrated as indicated by the baseline drawn under the peaks. Make changes in the Peak Threshold value or in the Peak Width setting and timed events for peak width adjustment in the method to fix most of these problems.

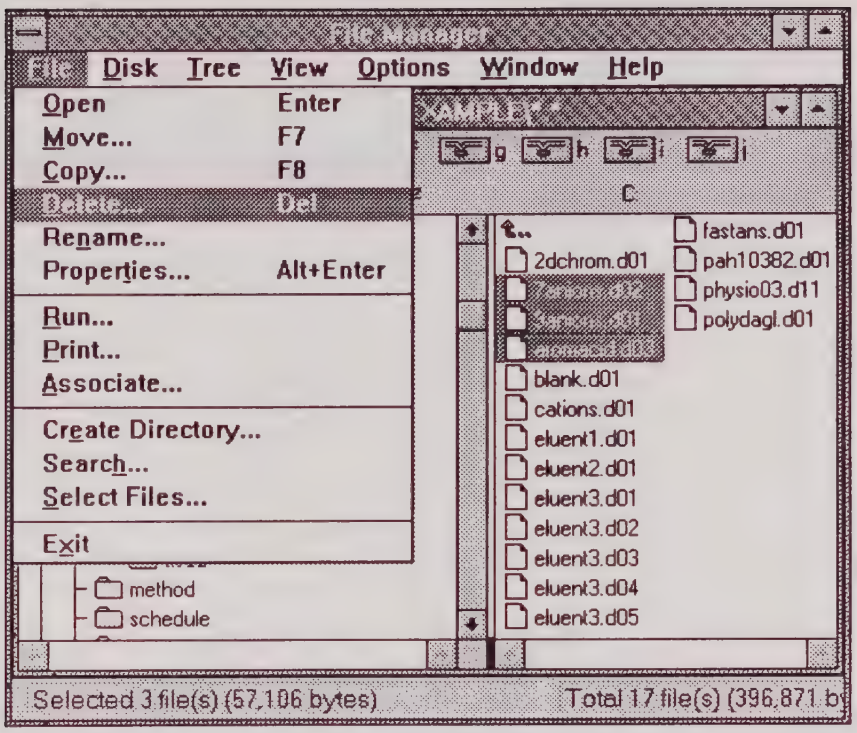


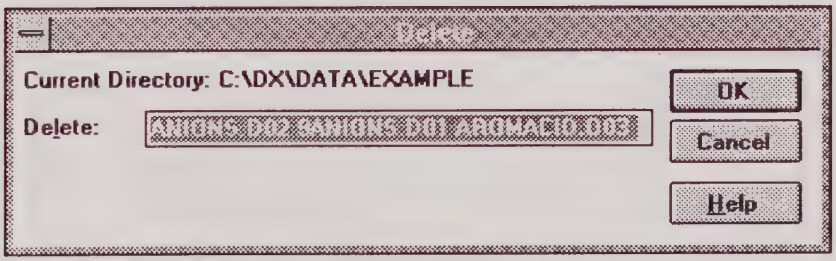
C. Deleting or Archiving Data Files

- even large hard disks fill up with data, method, and schedule files. These need to be removed to speed up processing and to allow for more storage space.

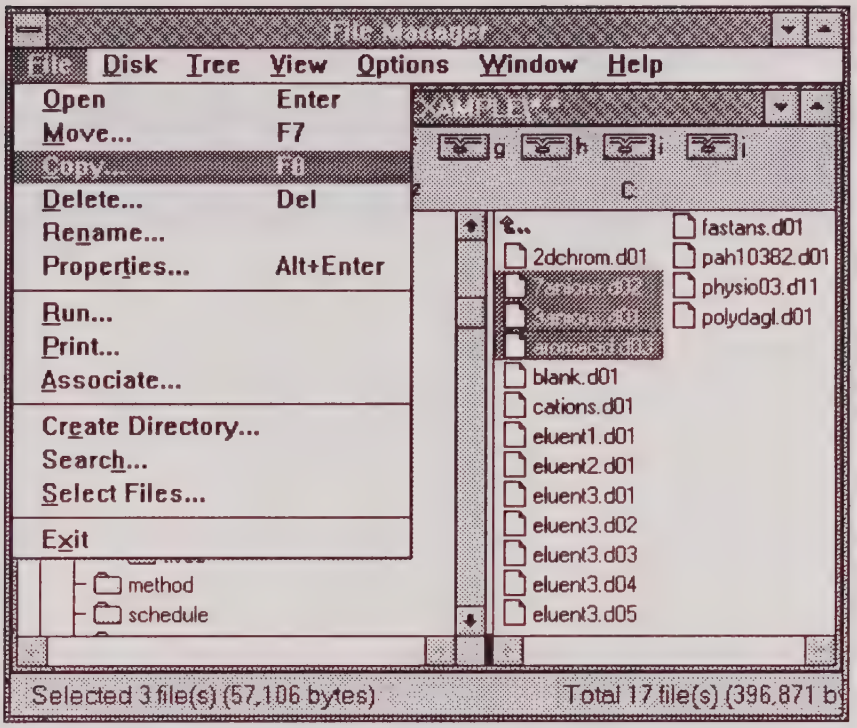
1. Use File Manager to Delete Unwanted Files

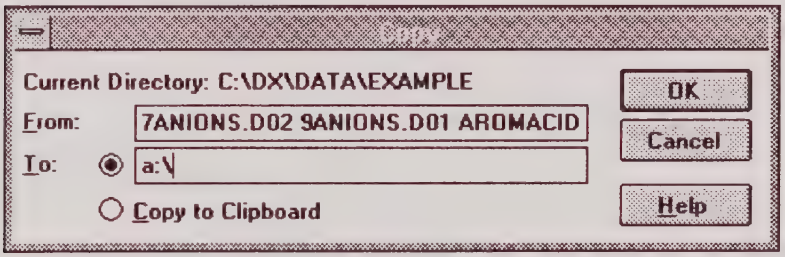




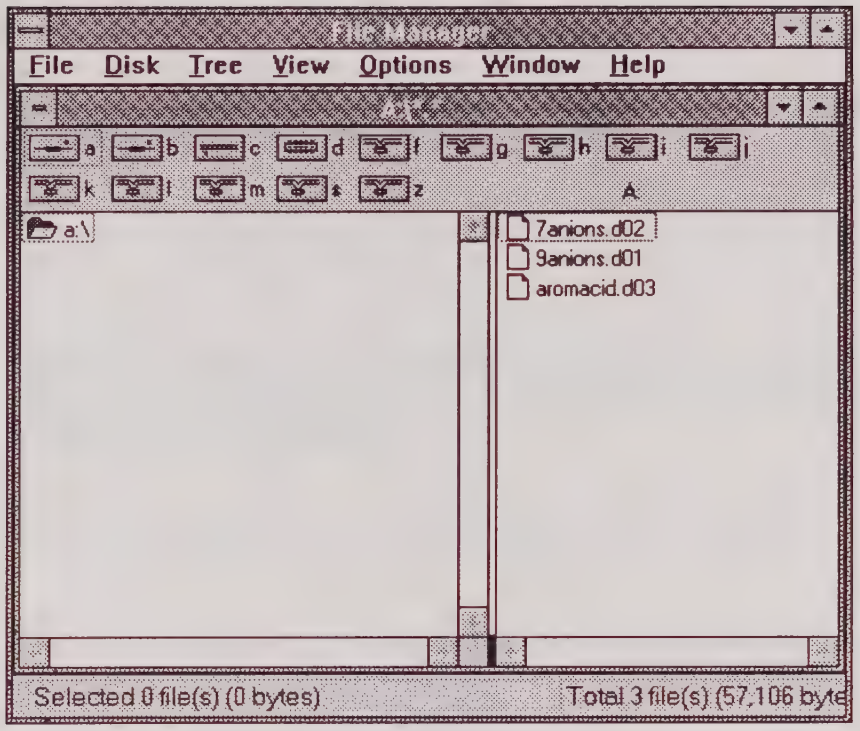


2. Use File Manager to Archive Data Files by Copying Them to a Floppy Disk in Drive A (or Drive B if available).





- Verify that the files have been copied to the floppy and then delete them from the hard disk.



D. Disk Maintenance

1. After Files Have Been Deleted, the Hard Disk is Fragmented.
   - Open spaces on disk in between other files
   - Remaining files may reside in non-contiguous sectors
   - Programs run slower because they must work with files which are spread out over the disk space.

2. Use Disk Compacting Programs to "Pack" Disk after Deleting Files.
   - PC Tools (Central Point Software, Inc., Beaverton OR) Compress Program
   - The Norton Utilities (SYMANTEC Corp., Cupertino, CA) Speed Disk Program
   - Others?

NOTE: **Dionex does not endorse or sell any of these utilities programs. The above list is for information only.**

EXERCISE 8

A. Examine one of the reports from the data you collected. Where is the data stored and which method file was used for the integration?

_____

_____

B. Inspect the chromatographic plot and determine if the peaks were integrated properly. What changes do you need to make in the method to properly integrate future chromatograms?

_____

_____

C. Copy the data files you generated from the standards and samples onto a floppy disk, supplied by your instructor. How do you know that they have been properly copied to the floppy disk?

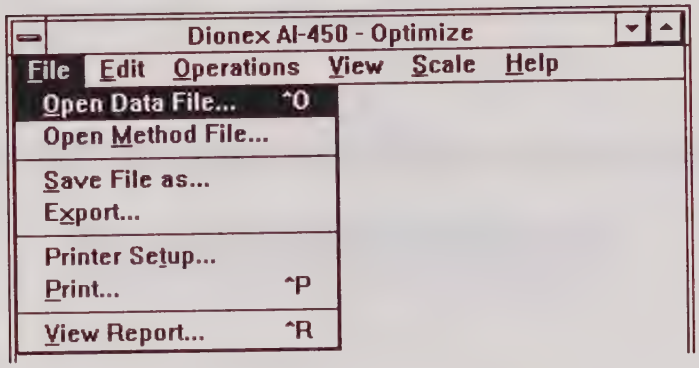
_____

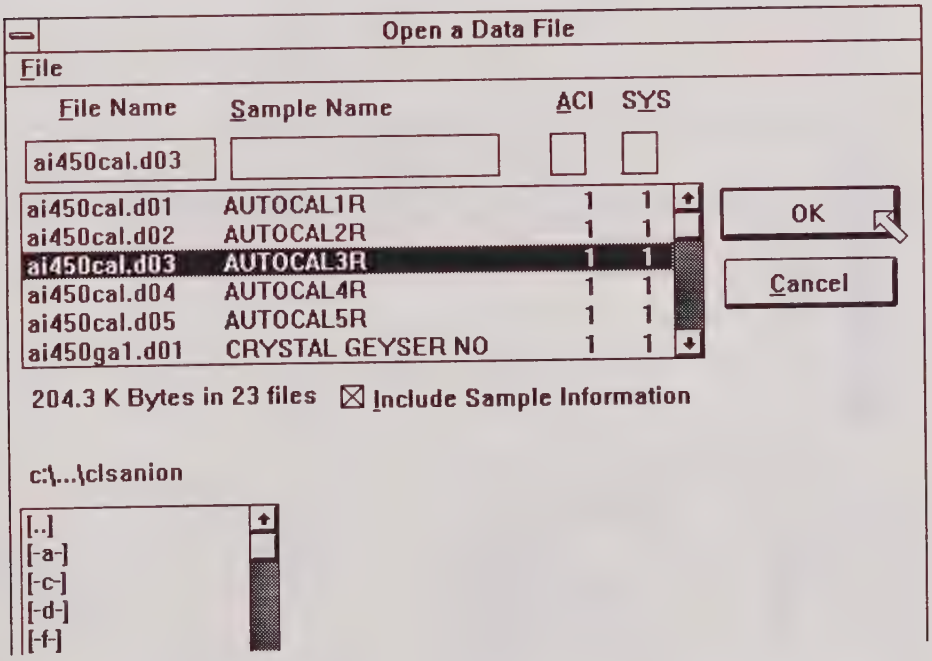
_____

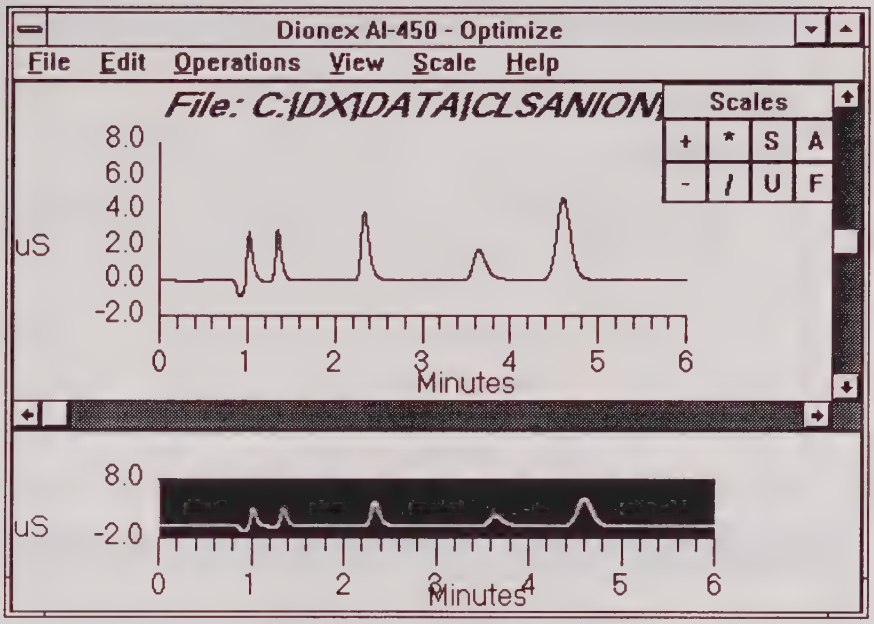
Delete these files from the hard disk after confirming that they are saved on the floppy disk.

VI OPTIMIZE-ing the Integration

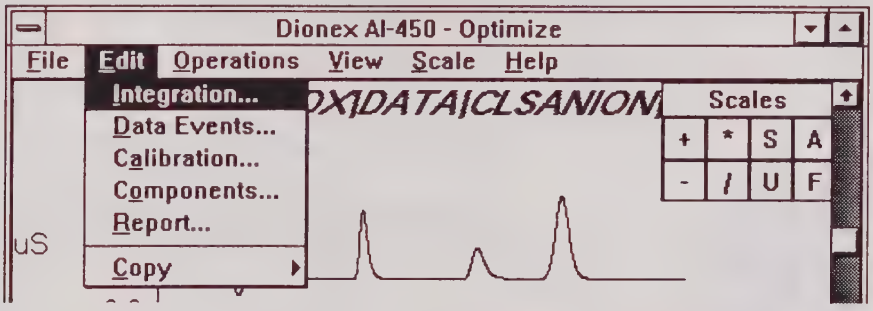
A. Getting Started with a Data File

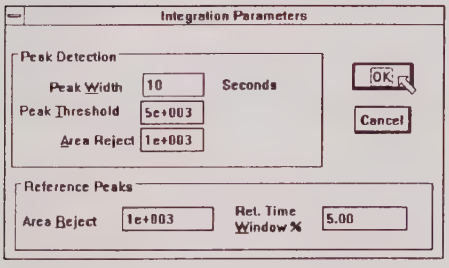


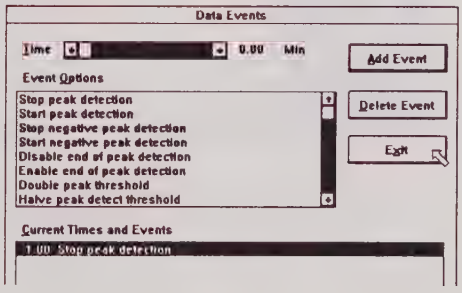


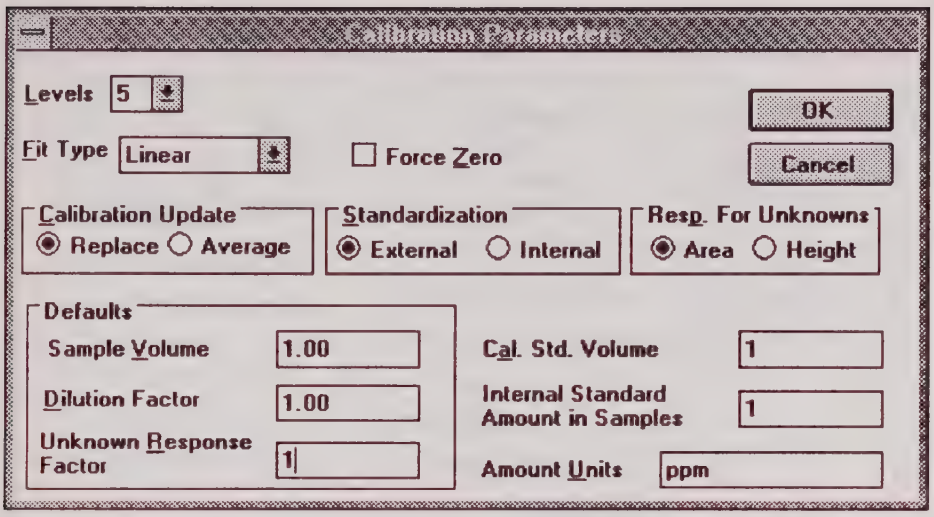


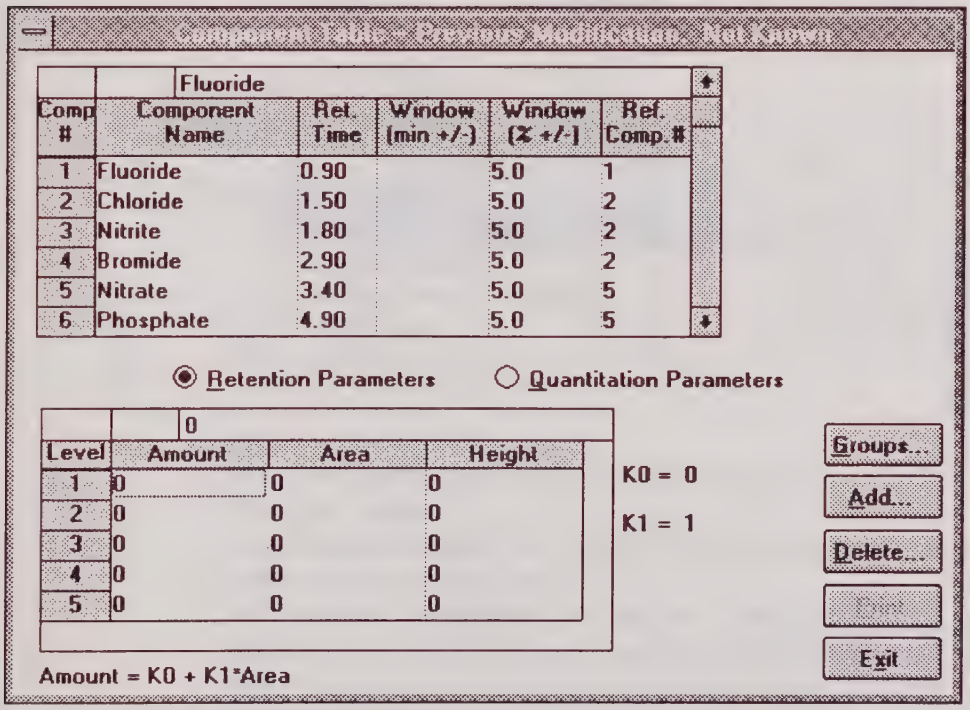
B. Editing the Method File

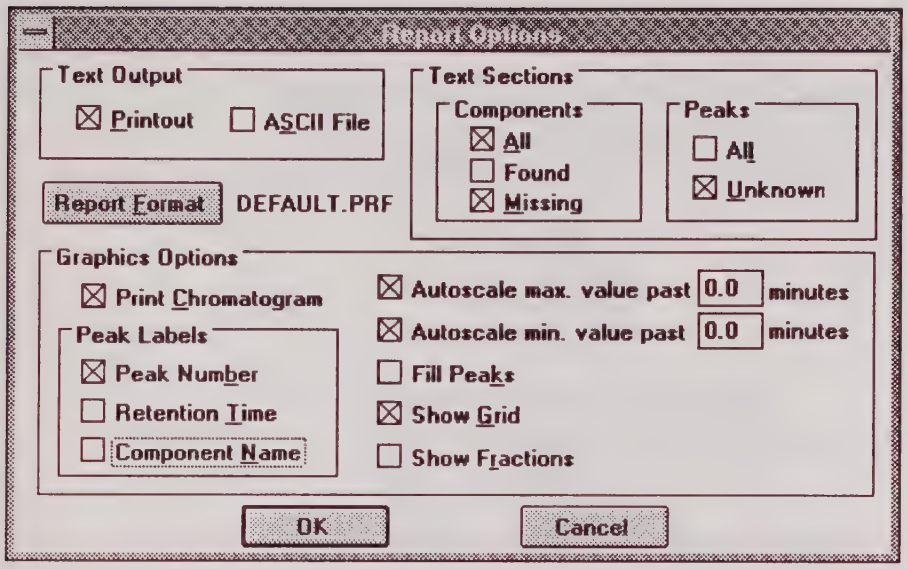




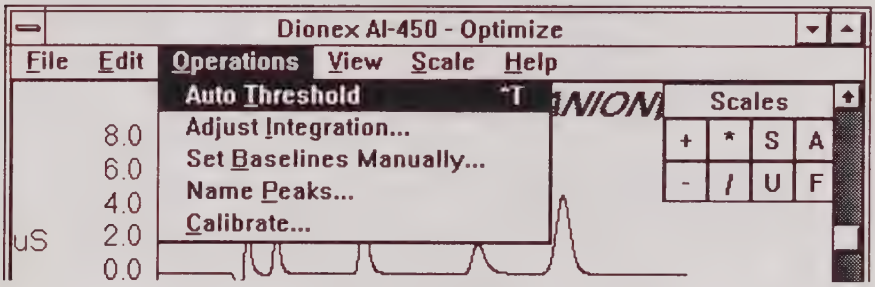



Calibration Parameters
Levels 5
Fit Type Linear
Force Zero
OK
Cancel
Calibration Update
Replace
Average
Standardization
External
Internal
Resp. For Unknowns
Area
Height
Defaults
Sample Volume 1.00
Dilution Factor 1.00
Unknown Response Factor 1
Cal. Std. Volume 1
Internal Standard Amount in Samples 1
Amount Units ppm


Fluoride
Comp # | Component Name | Ret. Time | Window (min +/-) | Window (% +/-) | Ref. Comp. #
1 Fluoride 0.90 5.0 1
2 Chloride 1.50 5.0 2
3 Nitrite 1.80 5.0 2
4 Bromide 2.90 5.0 2
5 Nitrate 3.40 5.0 5
6 Phosphate 4.90 5.0 5
Retention Parameters
Quantitation Parameters
0
Level | Amount | Area | Height
1 0 0 0
2 0 0 0
3 0 0 0
4 0 0 0
5 0 0 0
K0 = 0
K1 = 1
Groups...
Add...
Delete...
Exit
Amount = K0 + K1*Area



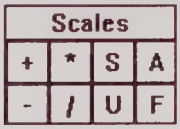
C. Operations of OPTIMIZE



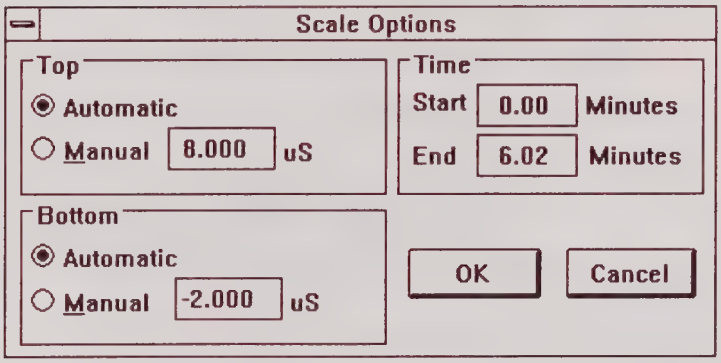
1. **Auto Threshold** measures baseline noise and recommends a Peak Threshold value.
2. **Adjusting Integration** calls up a window which allows timed events entries using graphics tools.
3. **Set Baselines Manually** allows the chromatographer to tell the computer exactly where to start and stop peak integration.
4. **Name Peaks** is a graphic tool to name the peaks found in the chromatogram.
5. **Calibrate** allows the updating of calibration information into the method after a calibration data file integration has been adjusted.

D. What to try first - Initial Values

- Before showing you how to manipulate the graphics part of the chromatogram, you need to know how to easily get back to the full chromatogram. This can be done using the **Scale Tools**.

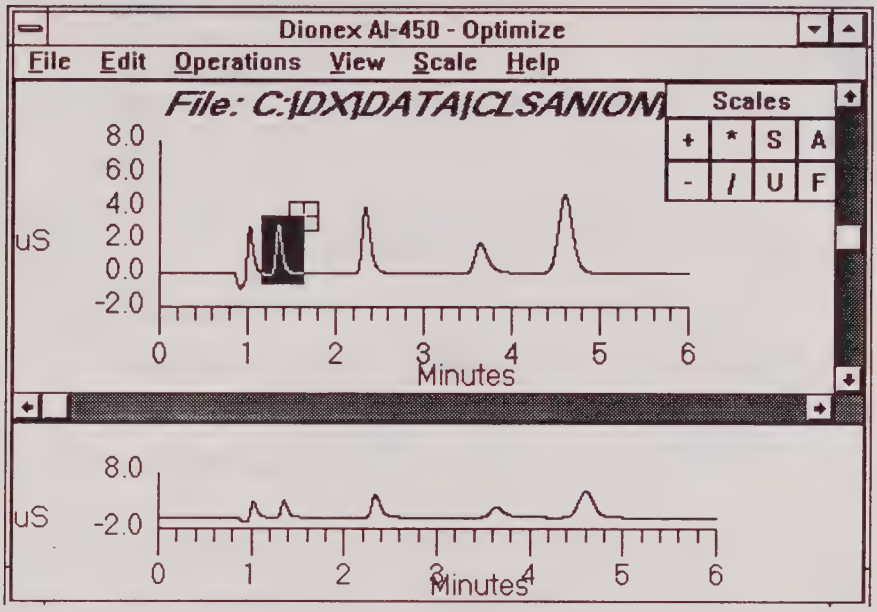


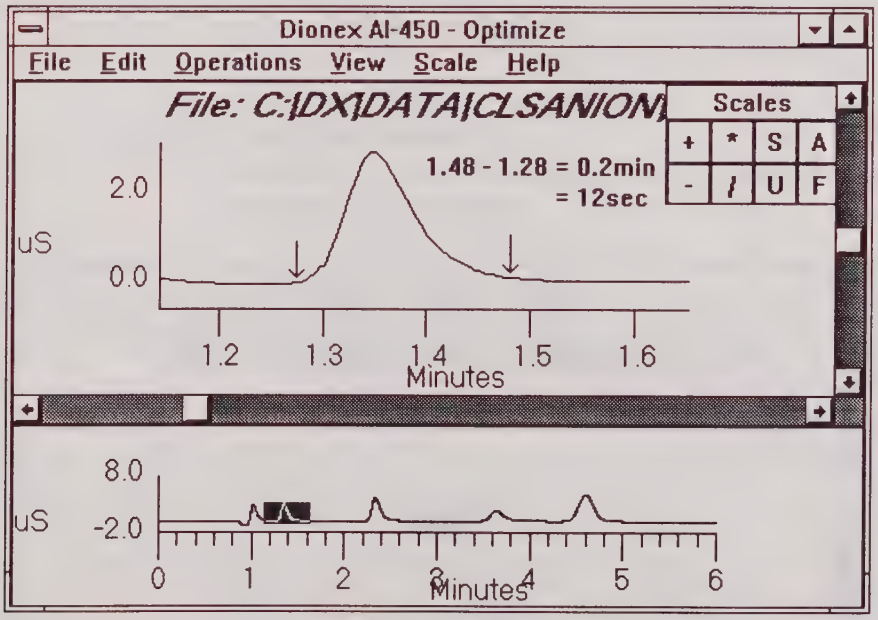
F restores the full scale chromatogram
U "undoes" the last scale change and allows you to toggle between two scales.
A autoscales the chromatogram.
S gives you quick access to the scale options:

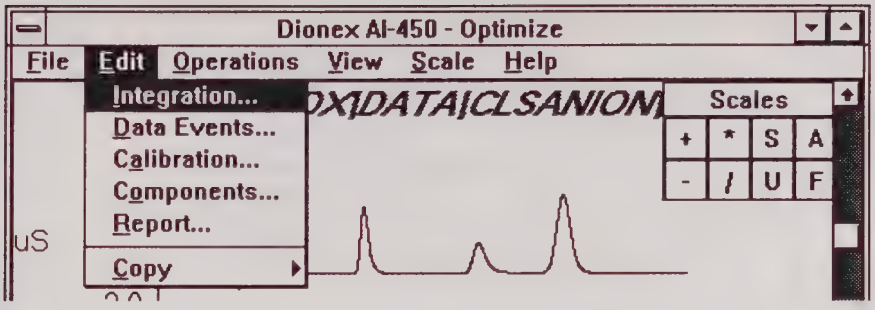


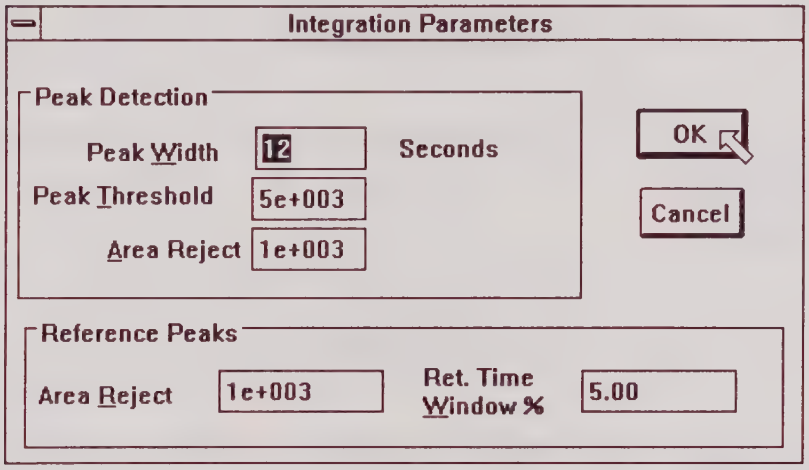
\+ zooms in vertically
\- zooms out vertically
* zooms in horizontally
/ zooms out horizontally

1. Measuring Peak Widths
   - Select an early peak and measure its baseline width.

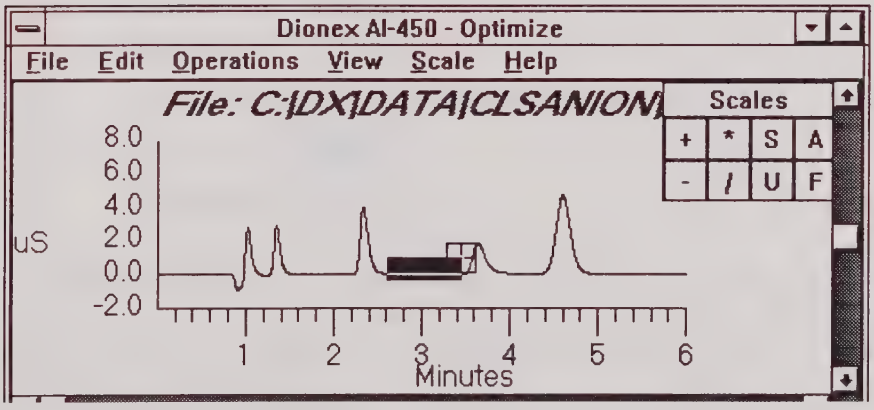


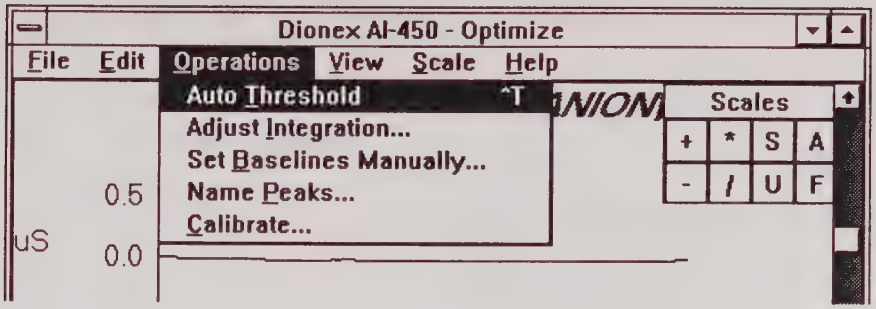


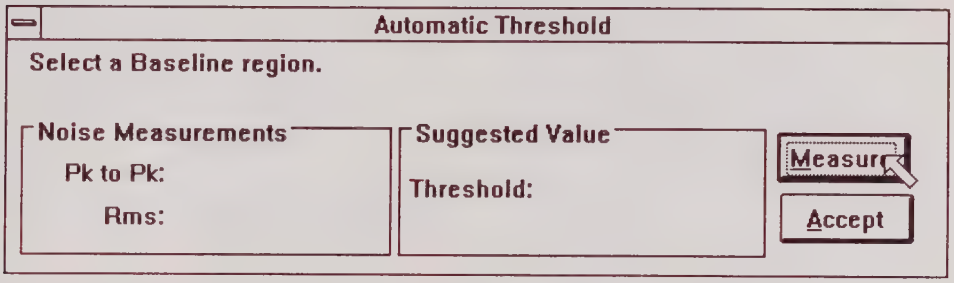


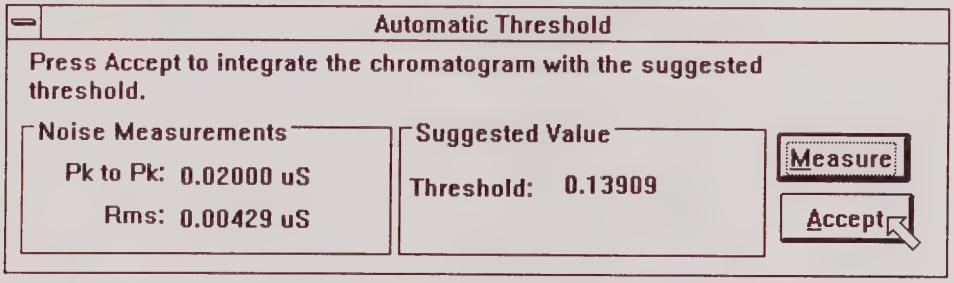


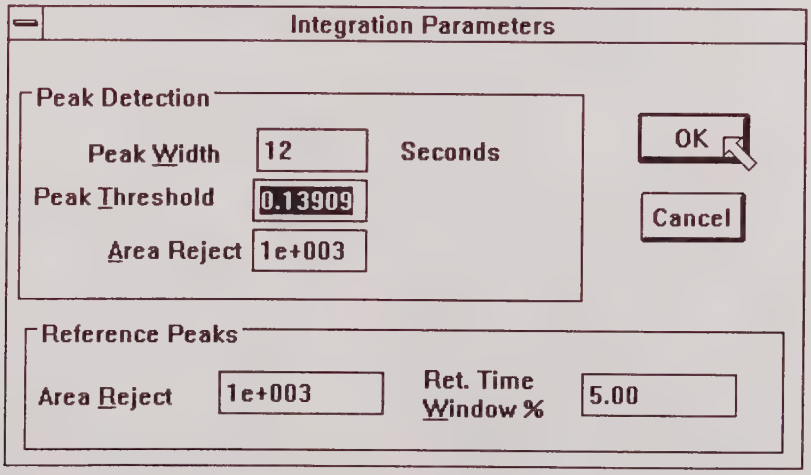
2. AutoThreshold Measurements
   - Select a baseline region and use the Auto Threshold Operation to measure the noise level.




Dionex AI-450 - Optimize
File Edit Operations View Scale Help
Auto Threshold ^T
Adjust Integration...
Set Baselines Manually...
Name Peaks...
Calibrate...
Scales
+ * S A
- / U F
0.5
uS
0.0


Automatic Threshold
Select a Baseline region.
Noise Measurements
Pk to Pk:
Rms:
Suggested Value
Threshold:
Measure
Accept

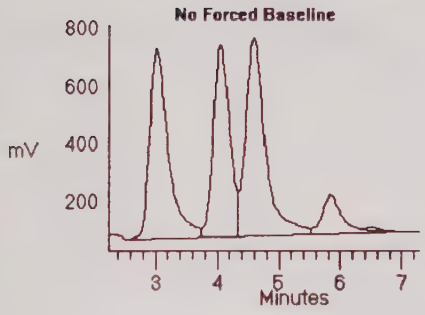

Automatic Threshold
Press Accept to integrate the chromatogram with the suggested threshold.
Noise Measurements
Pk to Pk: 0.02000 uS
Rms: 0.00429 uS
Suggested Value
Threshold: 0.13909
Measure
Accept

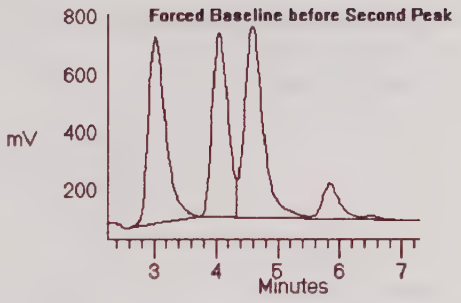

Integration Parameters
Peak Detection
Peak Width 12 Seconds
Peak Threshold 0.13909
Area Reject 1e+003
OK
Cancel
Reference Peaks
Area Reject 1e+003
Ret. Time Window % 5.00

E. What to try next - Data Events

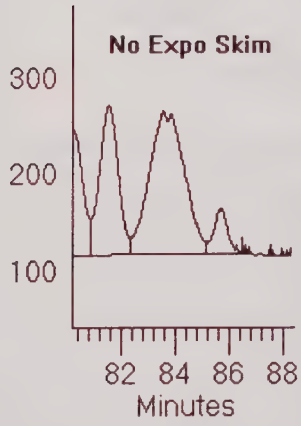
1. Description of Common Events:

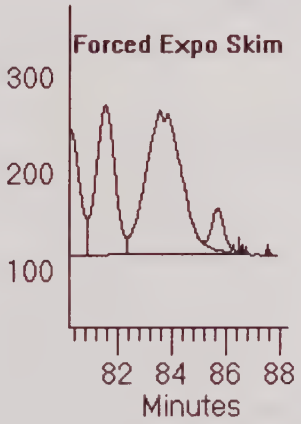
- Force Baseline



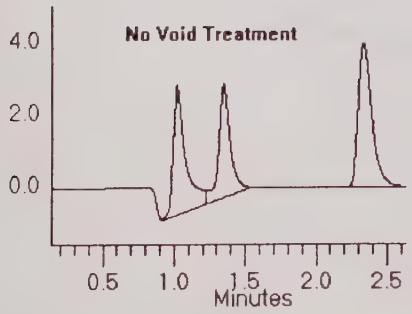


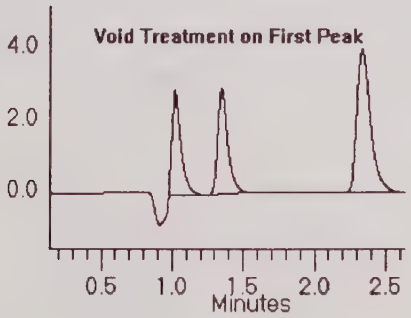
- Force Expo Skim





- Void Treatment

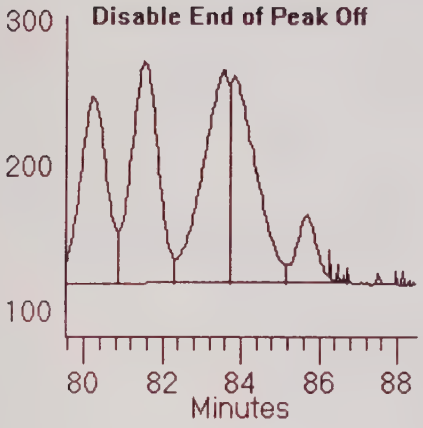


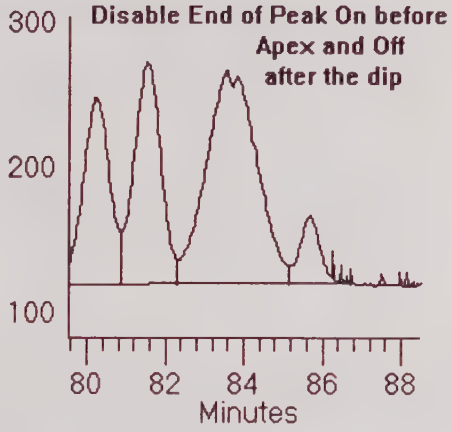


- Peak Detection: Turn peak detection off before unwanted peaks elute and back on after they elute.

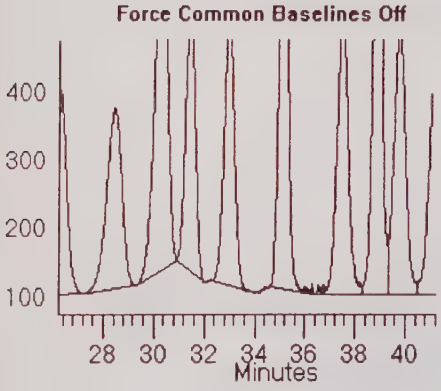
- **Negative Detection**: Allows the detection of negative peaks.

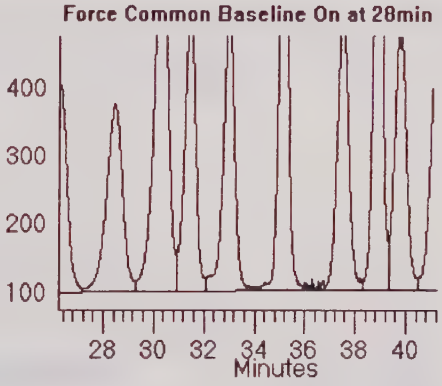
- **Disable End of Peak**





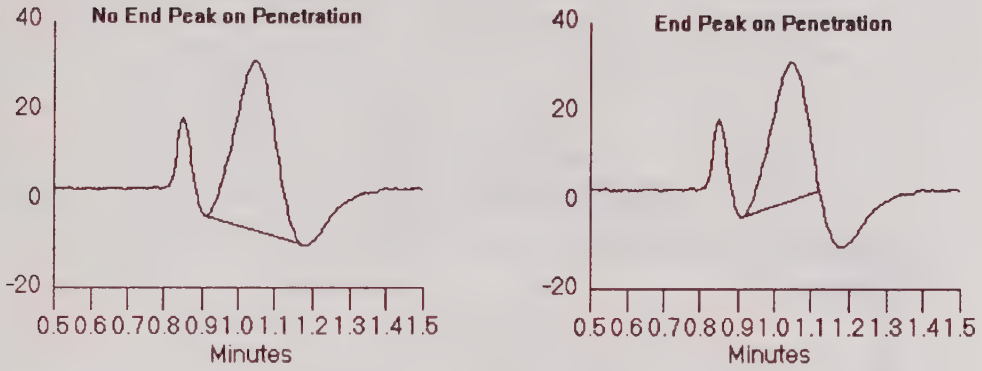
- **Force Common Baseline**





- **Force Separate Baseline**: The opposite of Force Common Baseline.

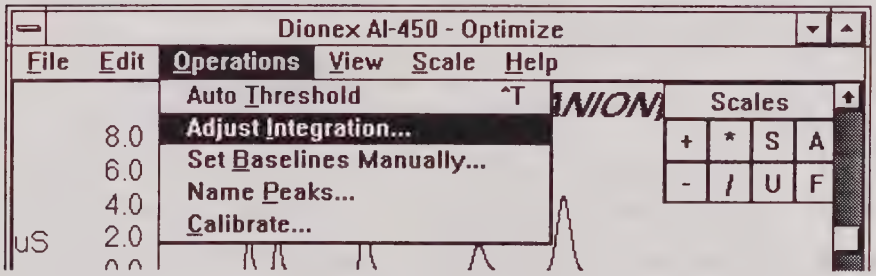
- **End Peak on Penetration:**

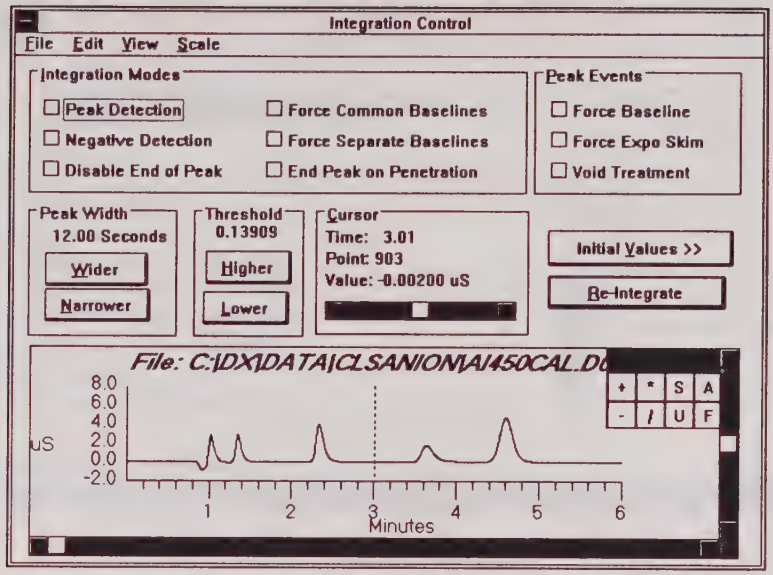


- **Peak Threshold:** Change Peak Threshold during the run to better integrate broad peaks (isocratic) or sharper peaks (gradient).

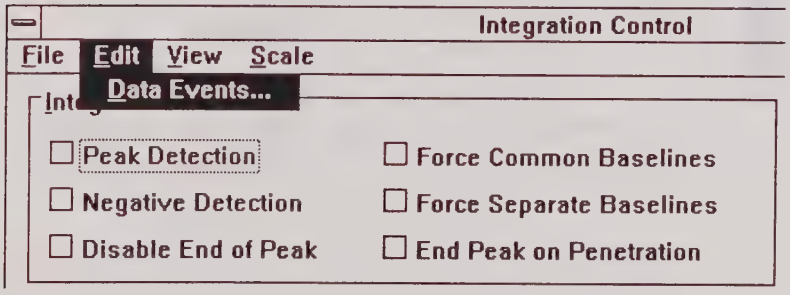
- **Peak Width:** Change Peak Width (Bunching Factor) during the run to better integrate broad peaks (isocratic) or sharper peaks (gradient).

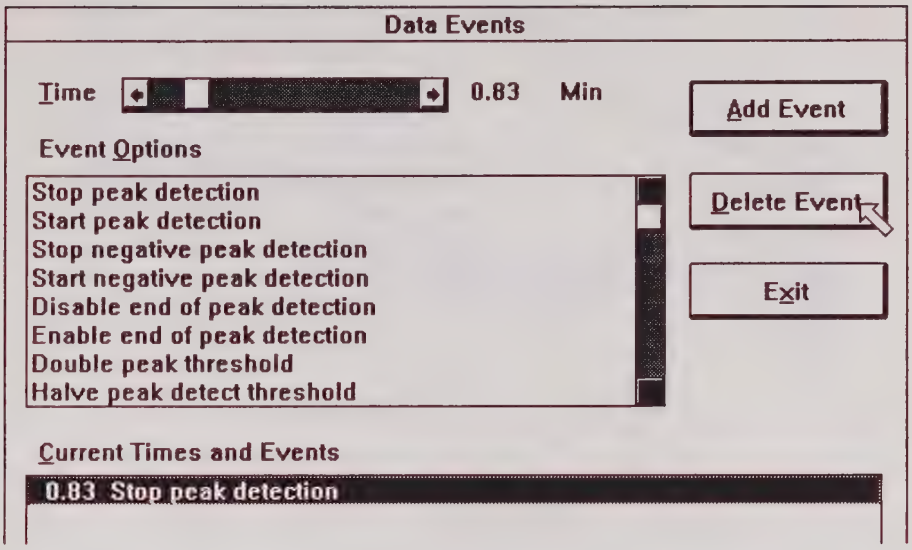
2. How to enter and test Timed Events





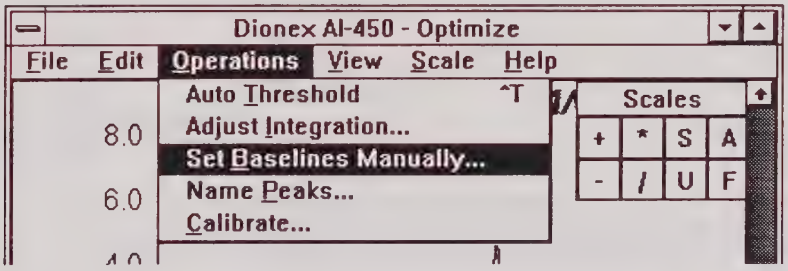
- Position cursor on chromatogram at bottom of Integration Control window at the time you want event to occur and click the **RIGHT HAND MOUSE BUTTON** to set the line cursor to that point.
- Click on the box next to the event you wish to add and the event will be added at the time indicated by the line cursor
- Test the effect of the timed event by clicking on the **Re-Integrate** button.
- Delete unwanted timed events by selecting the "Data Events" command from the **Edit** menu and deleting the event(s).



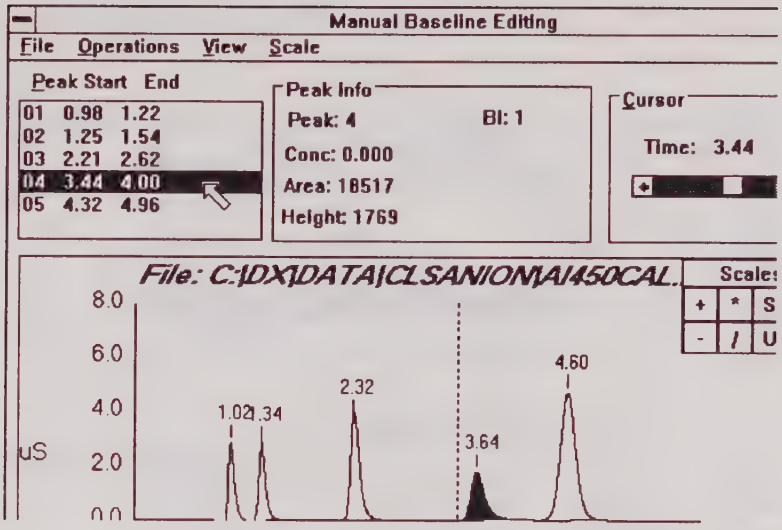


F. The last resort - Manual Baselines!

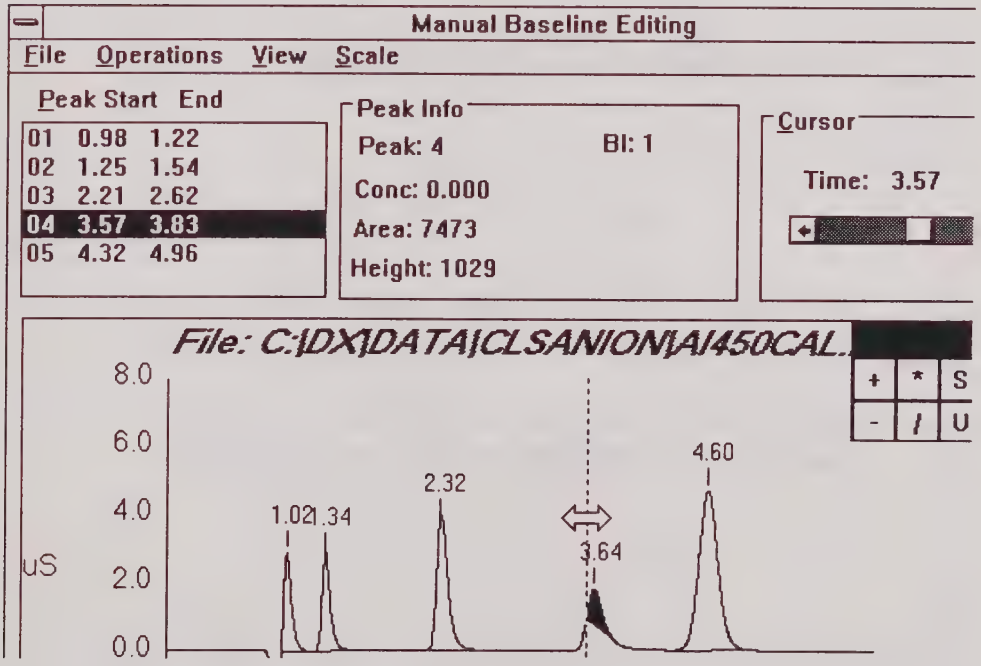
- only to be used when proper integration cannot be achieved using timed events
- NOT acceptable integration for Good Laboratory Practice (GLP)



- Select the peak you wish to manually integrate from the list of peaks in the upper left corner.

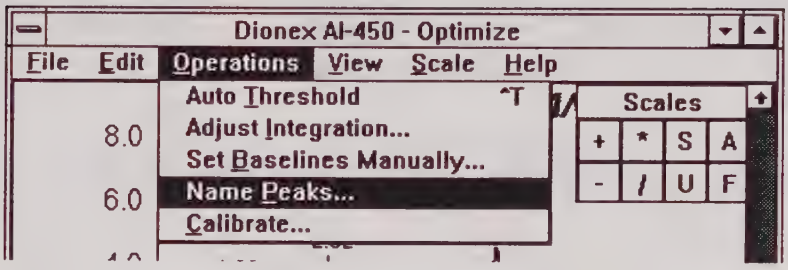


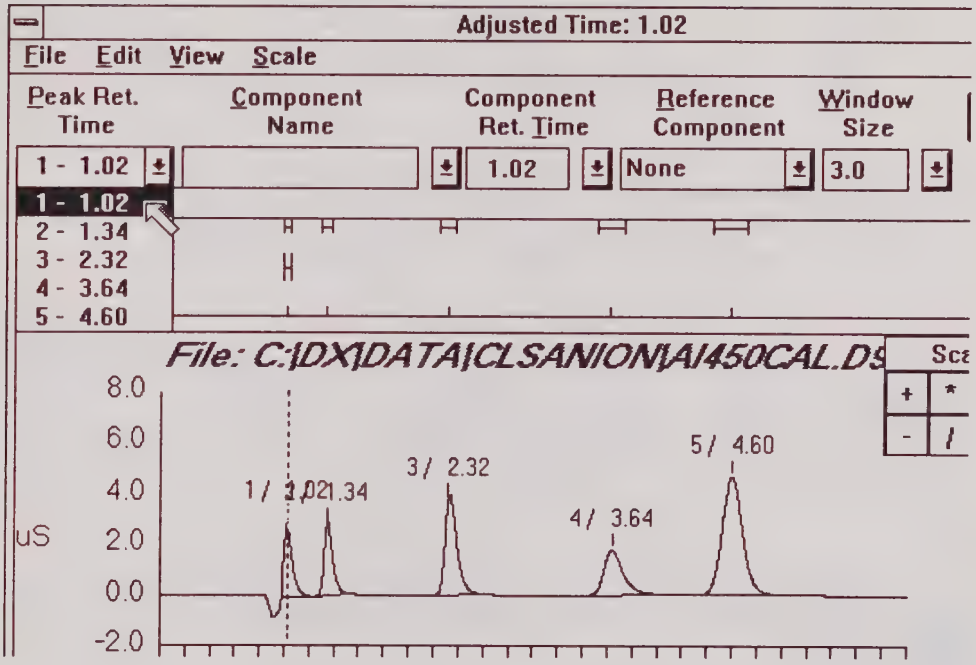
- Set the start and stop times by placing the mouse cursor on the chromatogram near the vertical line cursor, until it turns into a double arrow, and then drag the line cursor to the new start/stop location.



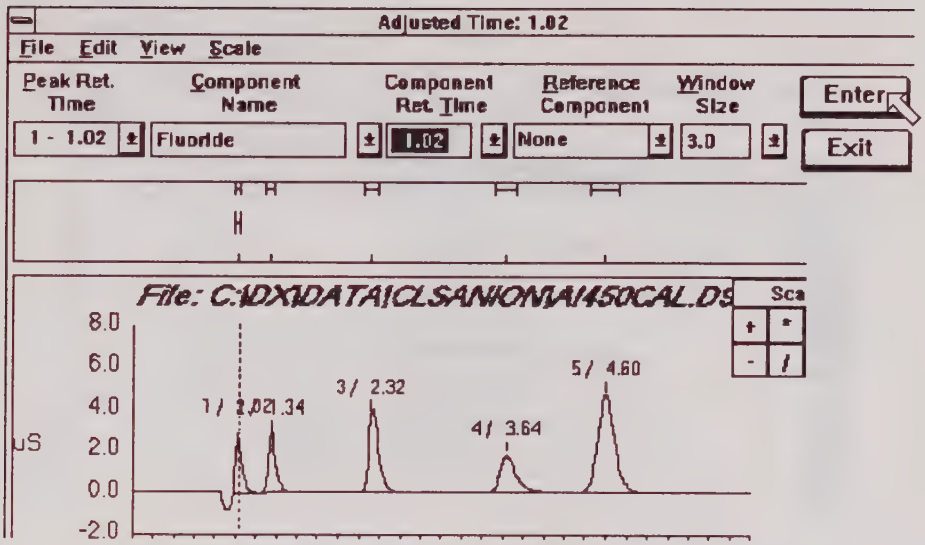
- Manual baselines can be saved when re-saving the chromatogram, but will be lost if the chromatogram is reintegrated.

G. Adjusting Named Peaks

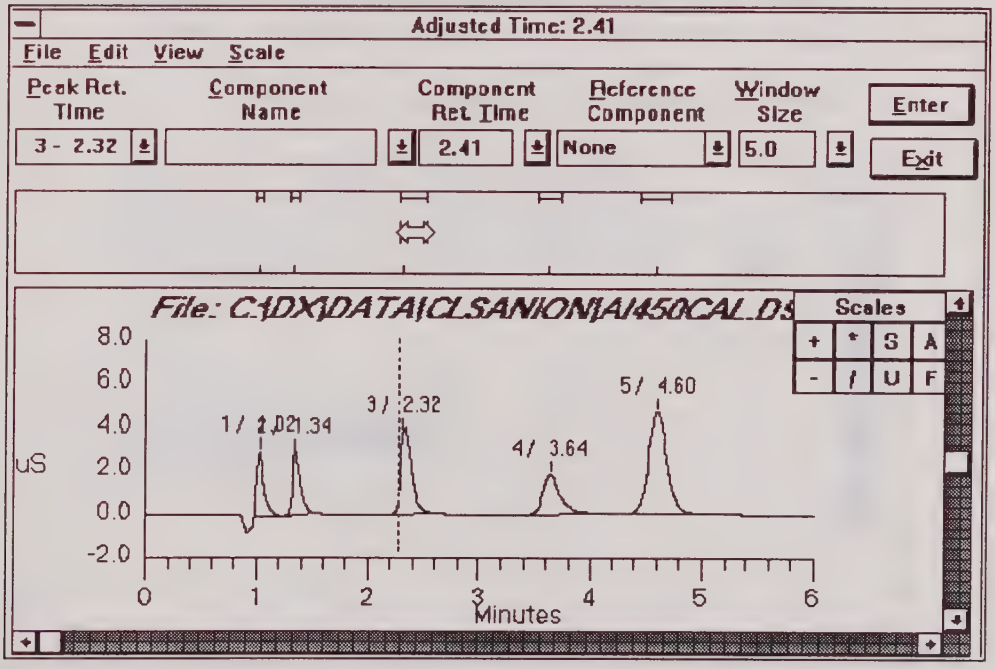




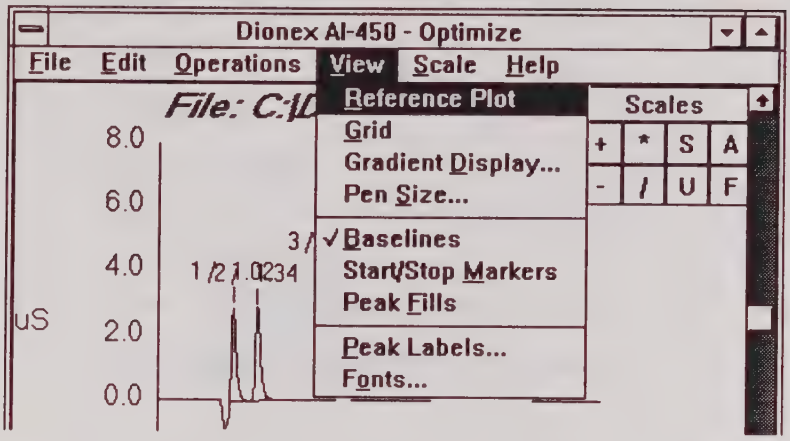
- Type in the name of the peak and press <TAB> to set the component retention time, and then press [ENTER] to enter the name.



- Move the peak detection window by clicking and dragging when the mouse arrow turns into a double arrow. Change the size of the window by entering another value for Window Size.

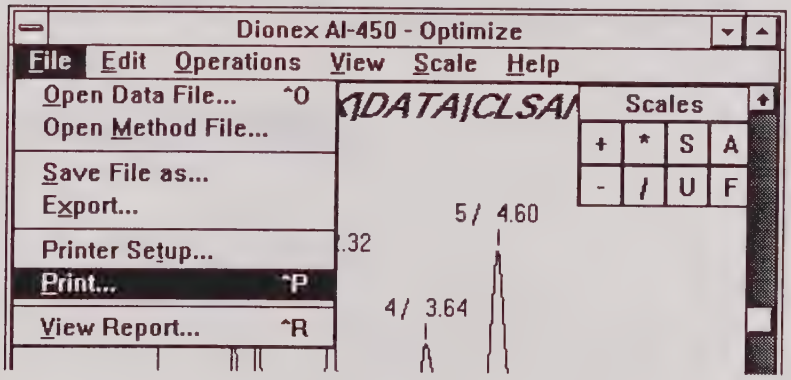


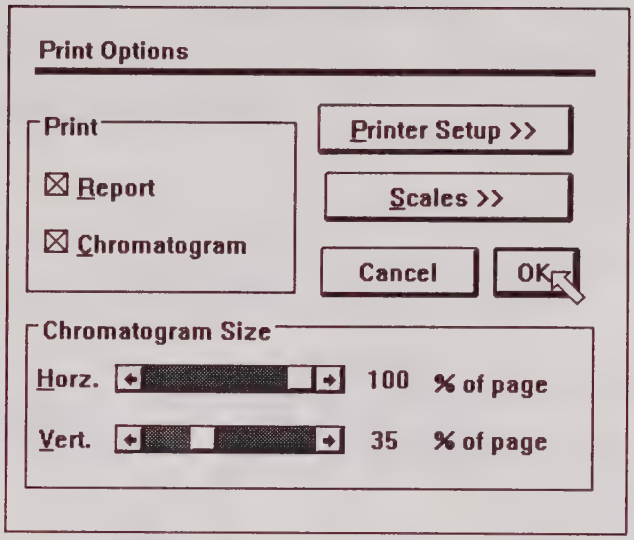
H. Customizing Graphics and Printout



- **Reference Plot** gives a full scale plot on the bottom of the window.
- **Grid** puts vertical and horizontal grid lines on the plot
- **Baselines** draws the baselines under all the peaks
- **Start/Stop Markers** show where the integration has been made
- **Peak Fills** color in the peaks for enhanced visual effects
- **Peak Labels** let you choose what isdisplayed about the peaks

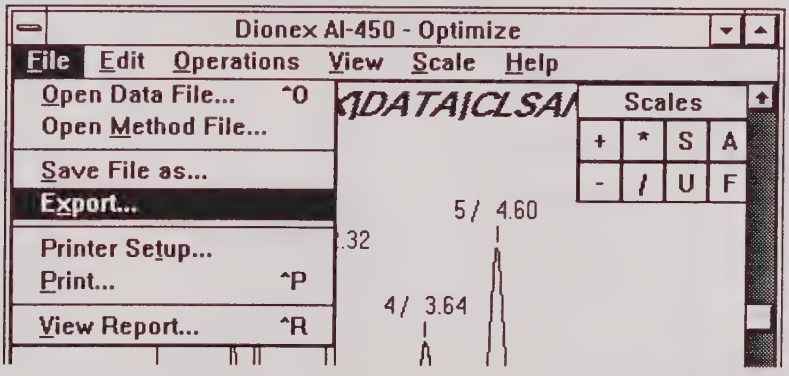
- Printout Parameters are accessed through the File Menu

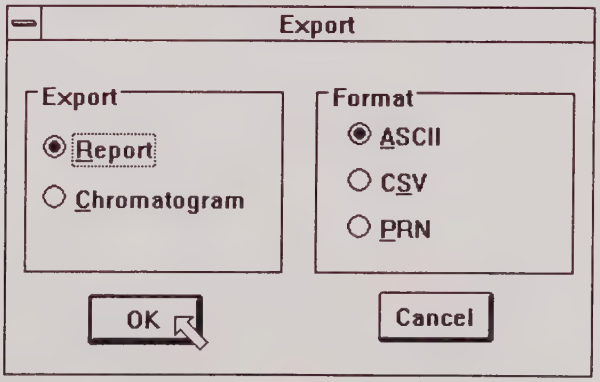


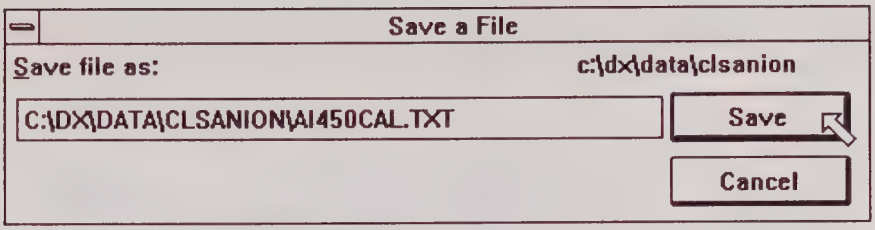


I. Exporting and Copying

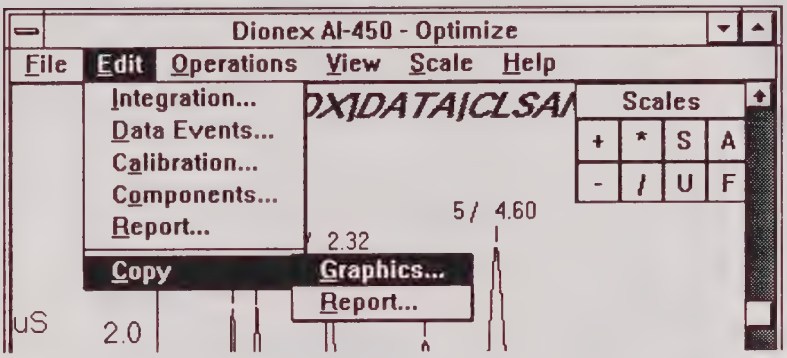
- Exporting the report or the chromatogram to a file is done through the File Menu **Export** command

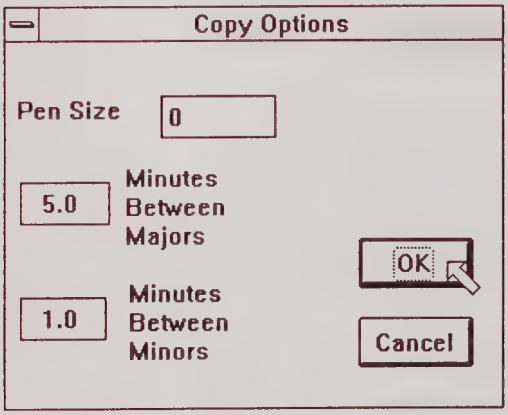




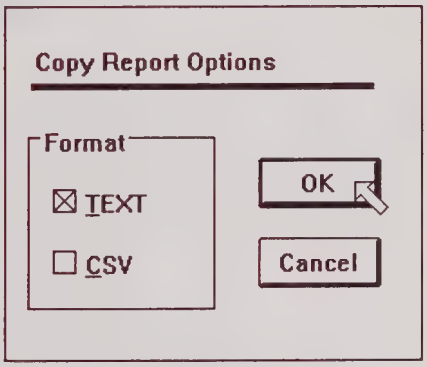


- Copying the chromatogram (Graphics) or Report to the Clipboard is done through the Edit Menu **Copy** command.



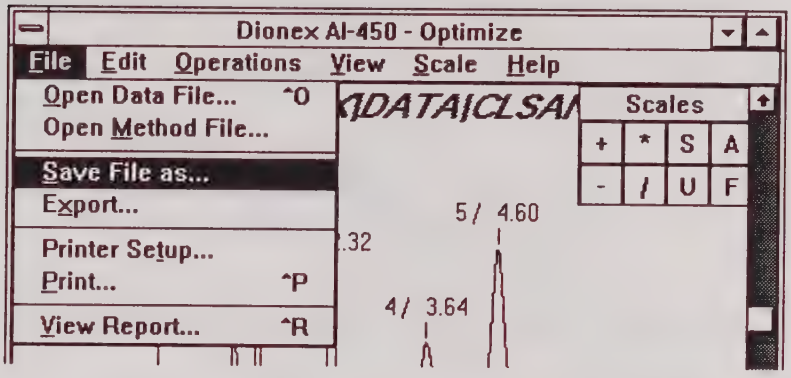


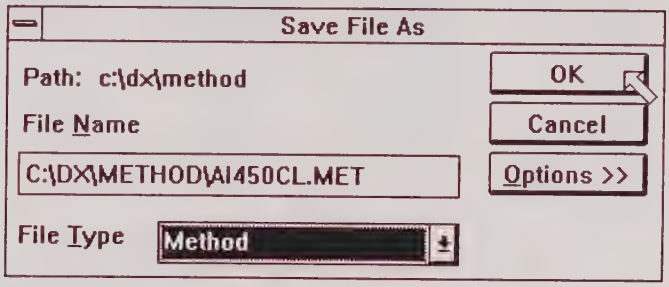
Copy Graphics to Clipboard



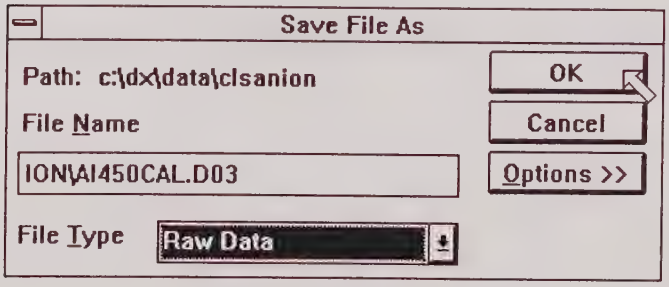
Copy Report to Clipboard

When Data File Has Been Properly Integrated and the Method "Fixed", BE SURE TO SAVE THE METHOD and maybe the Data File:





- Method information is stored with the Data File, so that when it is recalled, it is integrated in the same way. When you re-integrate the data file with OPTIMIZE and then save it, the "corrected" method information is stored with it. This needs to be done if you want the data file to be integrated "correctly" every time it is recalled.



EXERCISE 9

A. Optimize the AI450CAL.D03 chromatographic data file which you copied into the CLSANION subdirectory in Exercise 2.

1. Follow the recommended optimization procedure to integrate all peaks properly.
   a. Adjust initial conditions
   b. Establish Data Timed Events.
   c. Integrate using Manual Baselines (last resort!)

2. Name the peaks
3. Enter the following calibration information for all components:

Level	Fluoride	Chloride	Nitrate	Phosphate	Sulfate
1	0.4 ppm	0.6 ppm	2.0 ppm	3.0 ppm	3.0 ppm
2	1.0	1.5	5.0	7.5	7.5
3	2.0	3.0	10.0	15.0	15.0
4	5.0	7.5	25.0	37.5	37.5

4. Customize the printout
   a. Include grid
   b. Fill peaks
   c. Scale the chromatogram printout to 100% Horizontal x 50% Vertical.

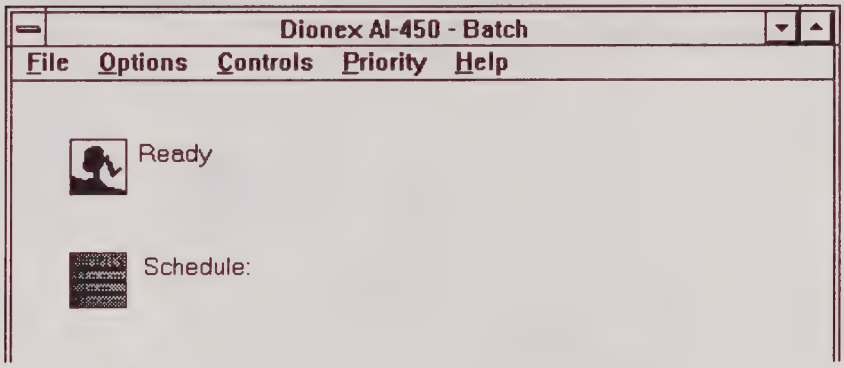
5. Save this optimized method as "OPTANION"

6. Save the optimized data file

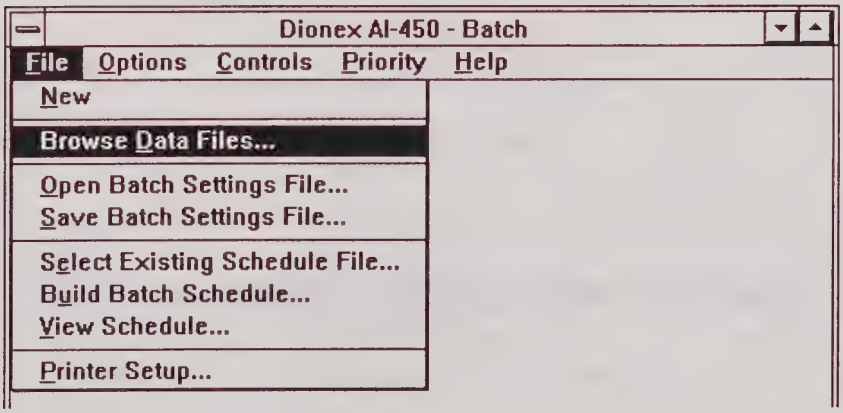
7. Recall this same data file and verify that it is now properly integrated.

VII. Optimizing Many Data Files with BATCH

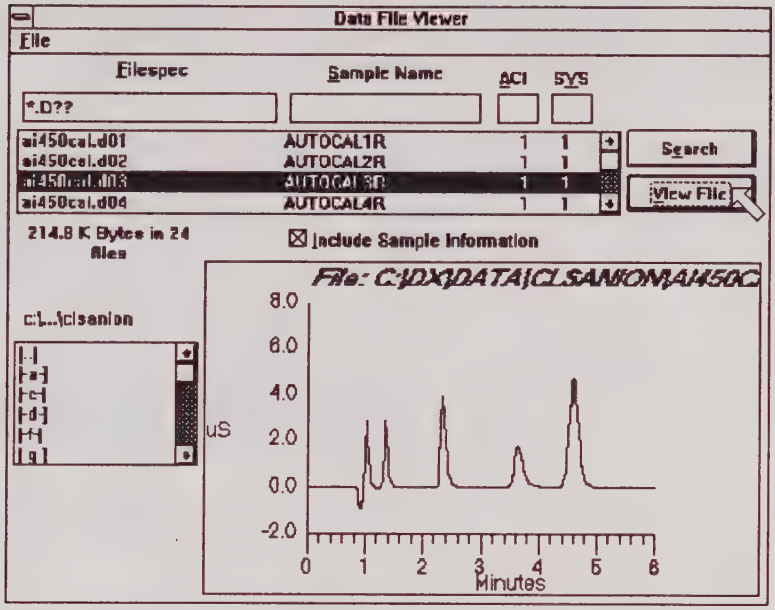
- BATCH is used to reintegrate many files at one time. This saves you from having to call them up one-by-one into OPTIMIZE just to reintegrate with a "fixed" Method.



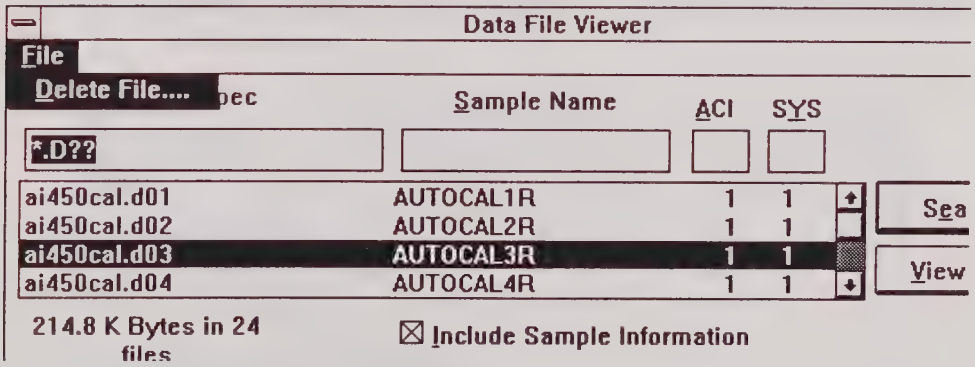
A. Browsing and Deleting Data Files



1. Select the file for previewing and click on the **"View File"** button

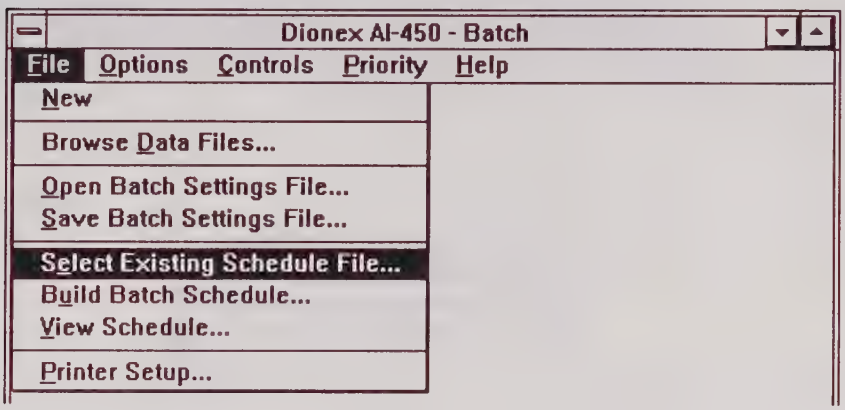


2. Delete chromatograms from this window using the File Menu **Delete File** command



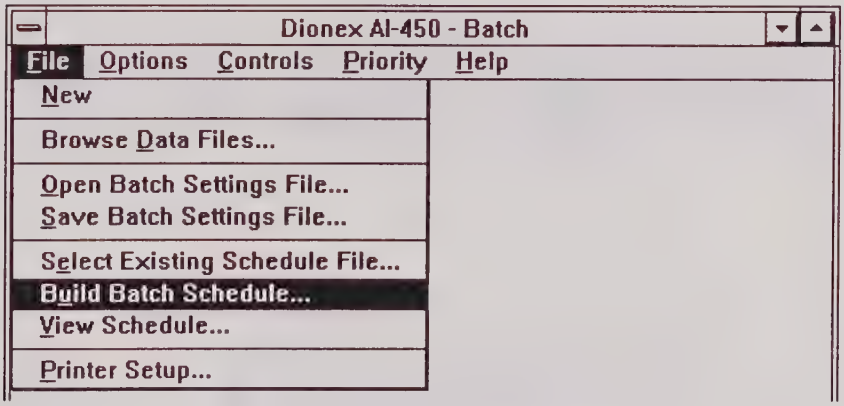
B. Building or Modifying a BATCH Schedule

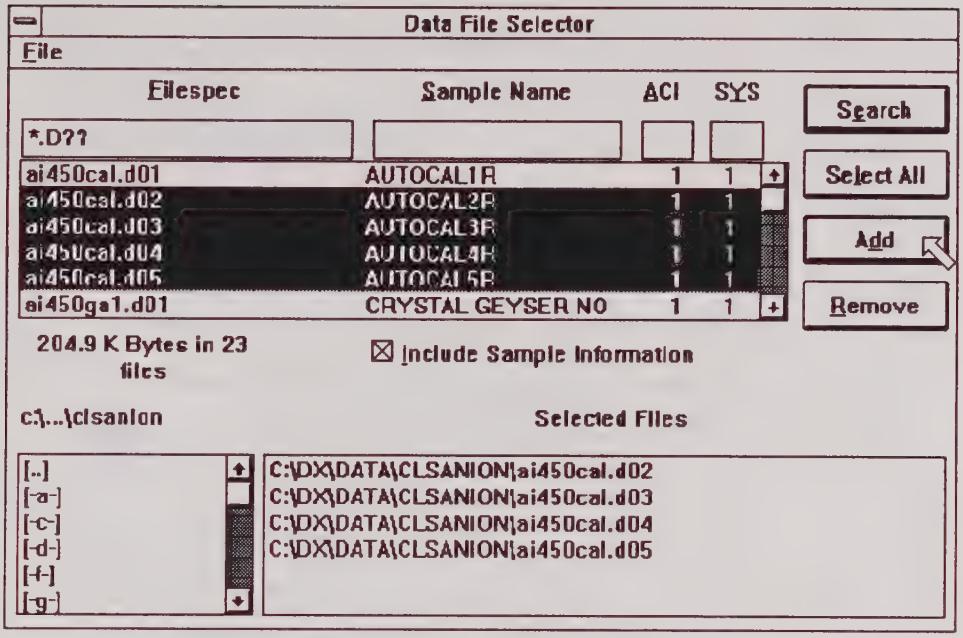
1. You can selecting an existing Schedule for Batch reintegration if all the data files in the schedule exist and match with their sample names.



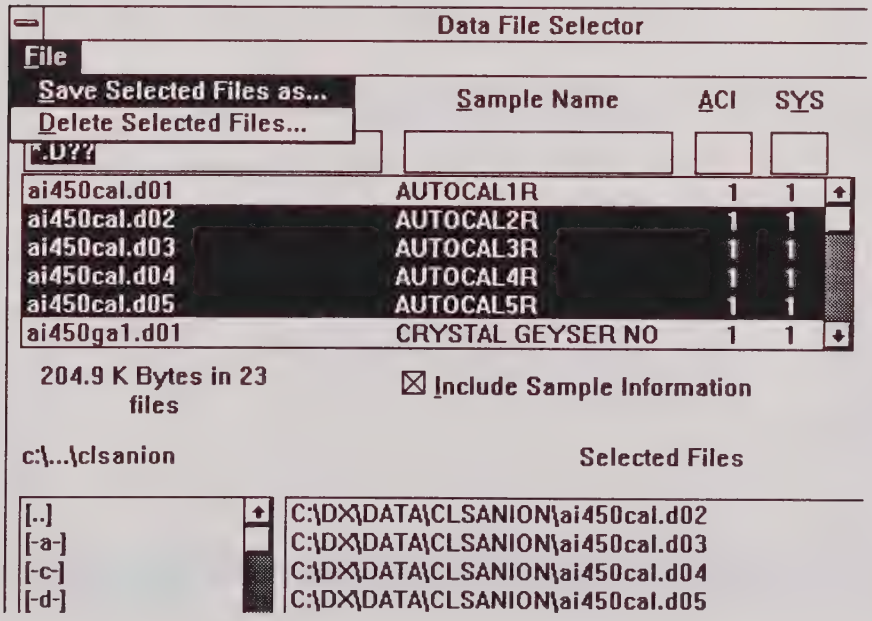
CAUTION - Data Files May Not Be Compatible

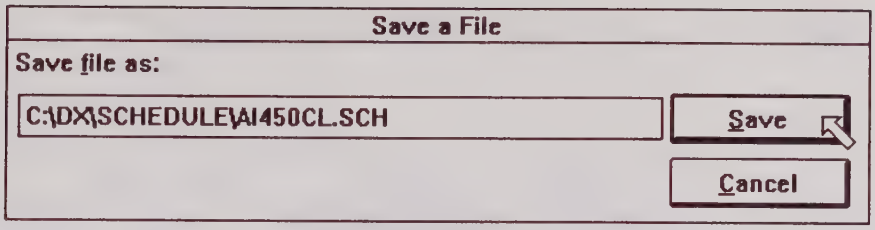
2. It is easy to build a Batch Schedule just by selecting the data files to be reintegrated



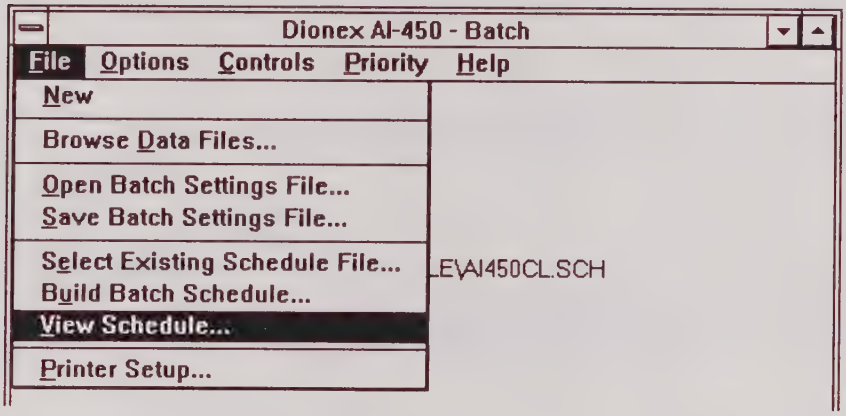


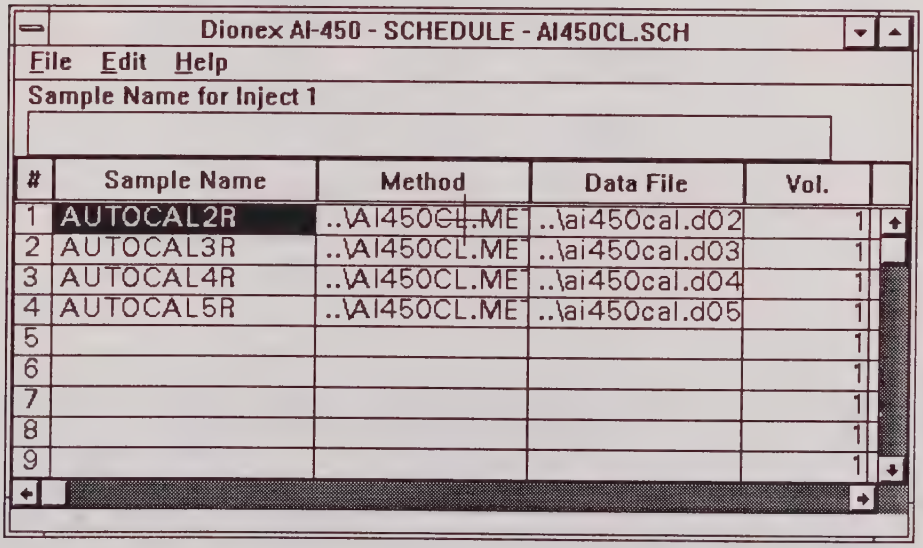
3. REMEMBER to save the selected files as a schedule file!



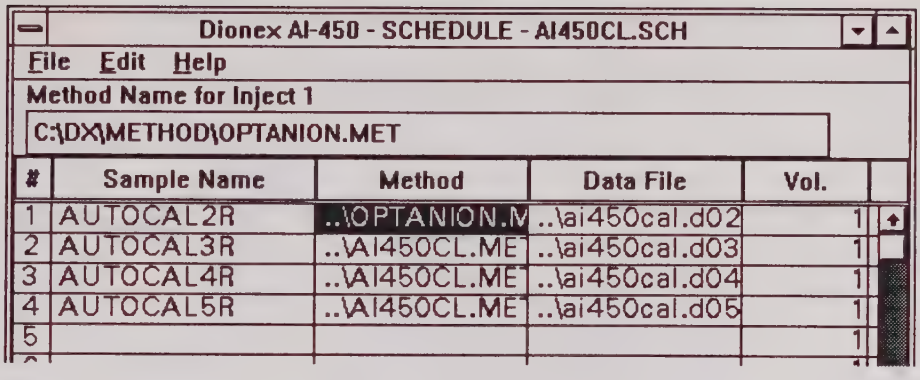


4. Next, view the schedule to make sure the method and data files and sample names are correct for what you want to batch reintegrate.

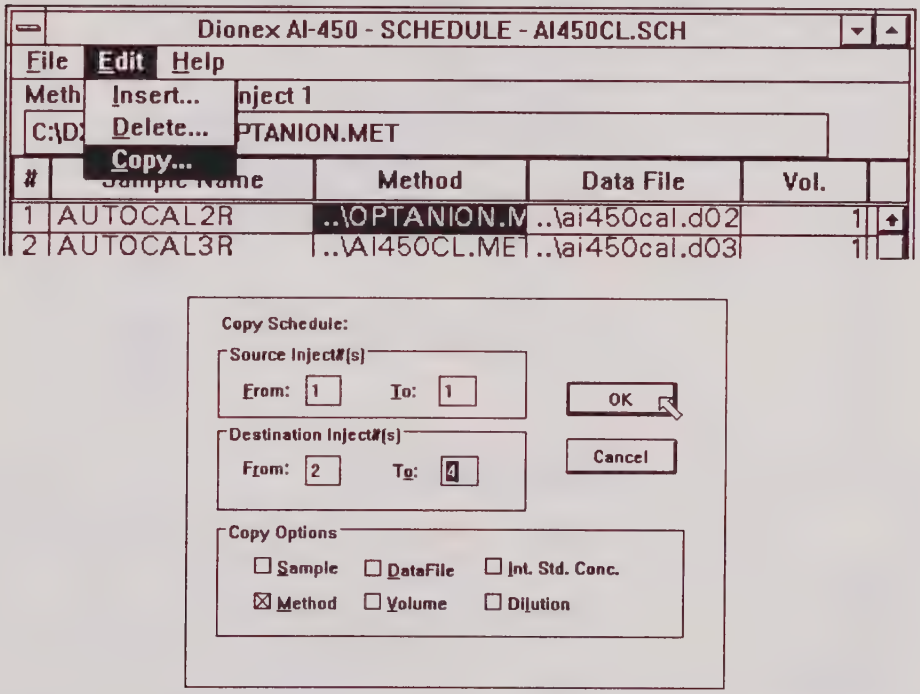


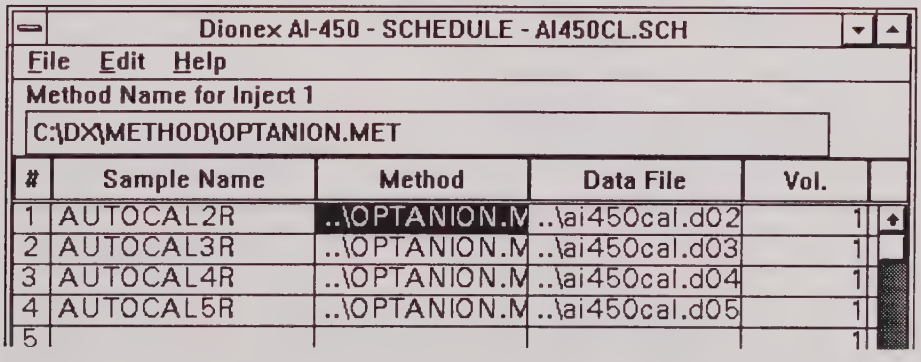


5. Click on the cell you want to change and then change it.

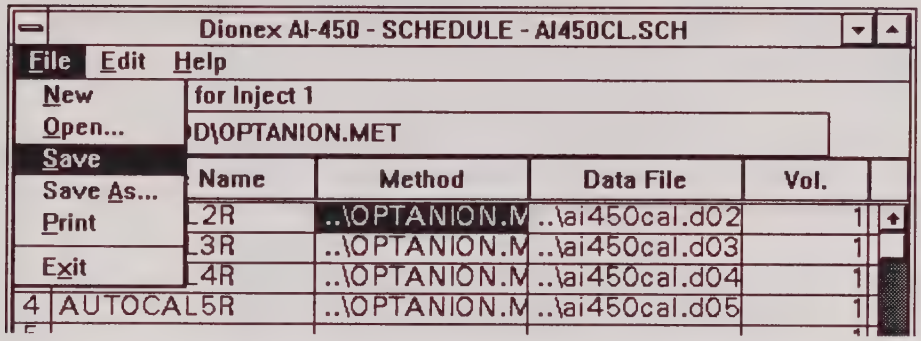

Dionex AI-450 - SCHEDULE - AI450CL.SCH
File Edit Help
Method Name for Inject 1
C:\DX\METHOD\OPTANION.MET
Sample Name Method Data File Vol.
1 AUTOCAL2R ..\OPTANION.M ..\ai450cal.d02 1
2 AUTOCAL3R ..\AI450CL.ME ..\ai450cal.d03 1
3 AUTOCAL4R ..\AI450CL.ME ..\ai450cal.d04 1
4 AUTOCAL5R ..\AI450CL.ME ..\ai450cal.d05 1
5 1

6. Then use the copy command to make multiple changes.

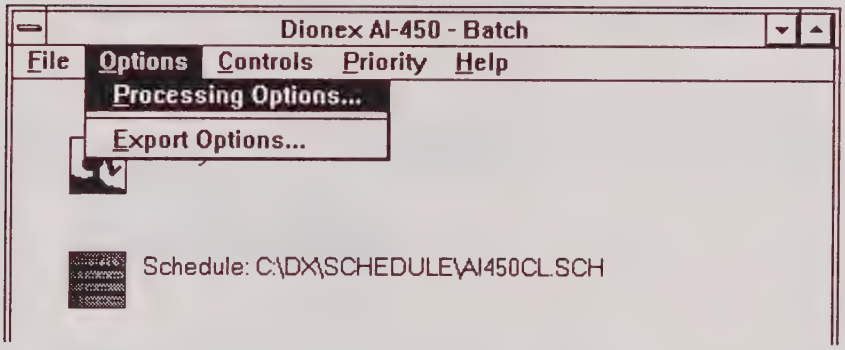


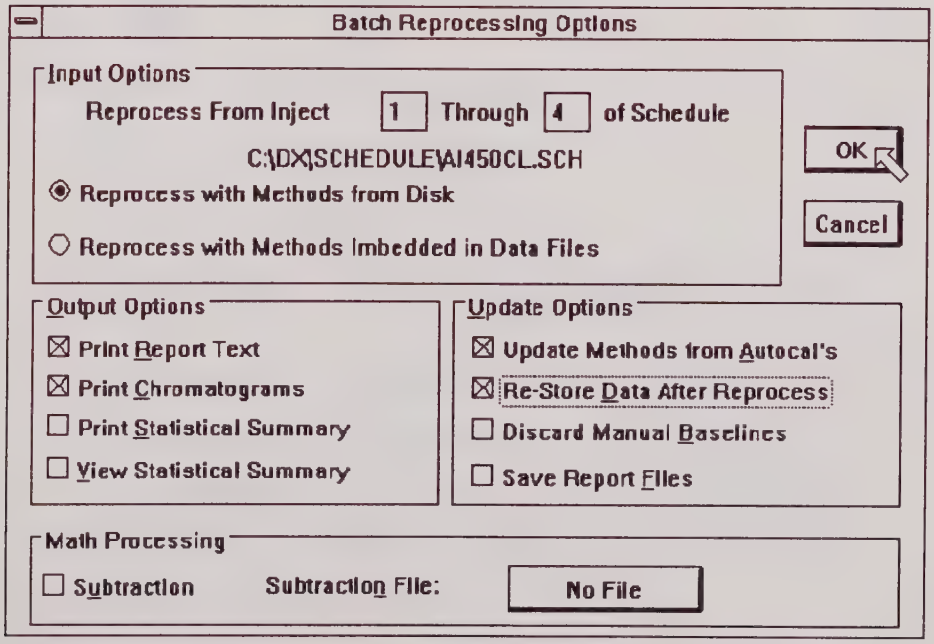

Dionex AI-450 - SCHEDULE - AI450CL.SCH
File Edit Help
Method Name for Inject 1
C:\DX\METHOD\OPTANION.MET
Sample Name Method Data File Vol.
1 AUTOCAL2R ..\OPTANION.M ..\ai450cal.d02 1
2 AUTOCAL3R ..\OPTANION.M ..\ai450cal.d03 1
3 AUTOCAL4R ..\OPTANION.M ..\ai450cal.d04 1
4 AUTOCAL5R ..\OPTANION.M ..\ai450cal.d05 1
5 1

7. Be sure to Save the modified schedule when you are finished!



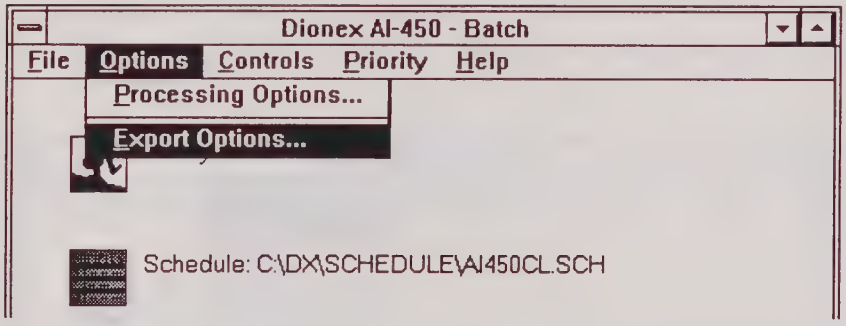
8. Next, you need to specify the Processing options you would like for the Batch reintegration.

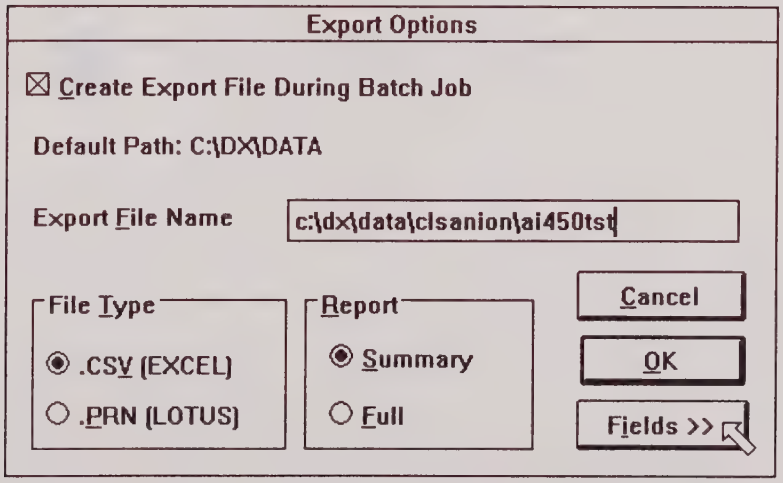


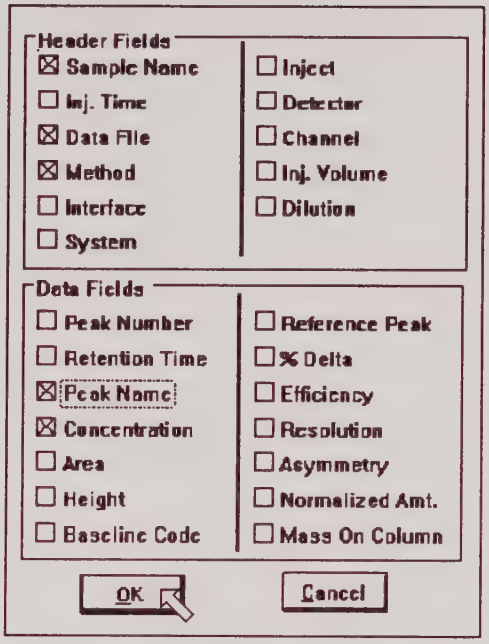


- **Input Options** let you specify which sequencial set of lines in the schedule to reprocess.
- **Output Options** let you choose what will be printed out and whether you want a Statistical report (for replicate samples only) printed or just viewed on the screen.
- **Update Options** let you select whether or not to update methods, restore the data file (with the new method information), throw out manual baselines for this reintegration, or save the report files in a test format.
- **Math Processing** allows the automatic subtraction of a file (like a blank) from all the data files being reprocessed.

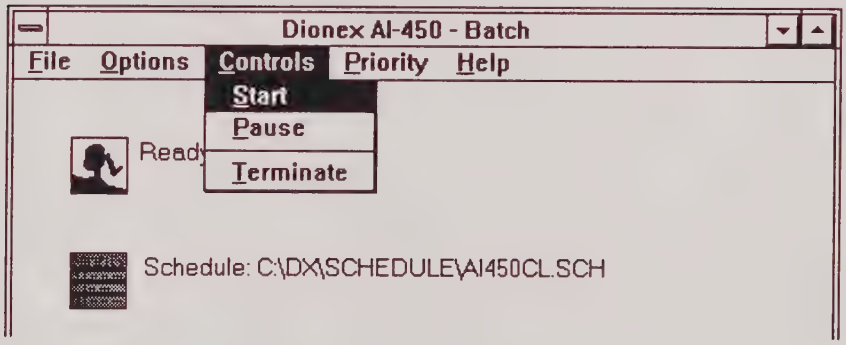
9. Then, specify any Export Options you would like for the reprocessing. Exporting means to send parts (or all) of the report to a EXCEL or LOTUS 123 file. You specify which parts by clicking on "Summary" and then selecting the desired fields in the "Fields" screen.







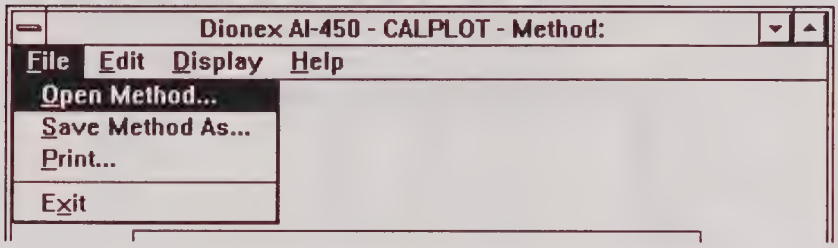
10. Lastly, you need to START the batch reprocession from the Control Menu.

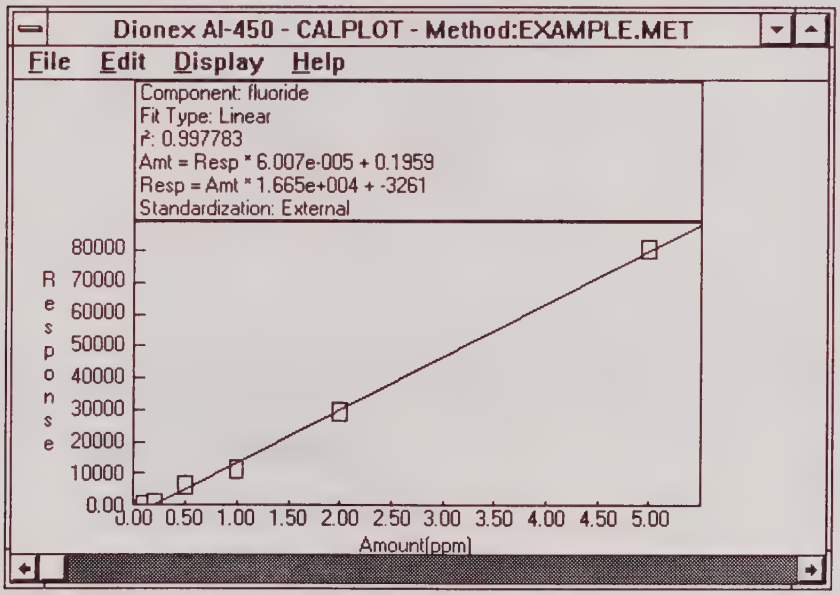


VIII. Viewing Calibrations with CALPLOT

A. Editing the Components or the Calibration

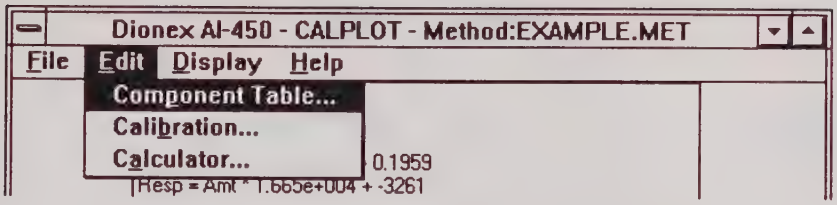
1. First, open the method where the calibration resides.

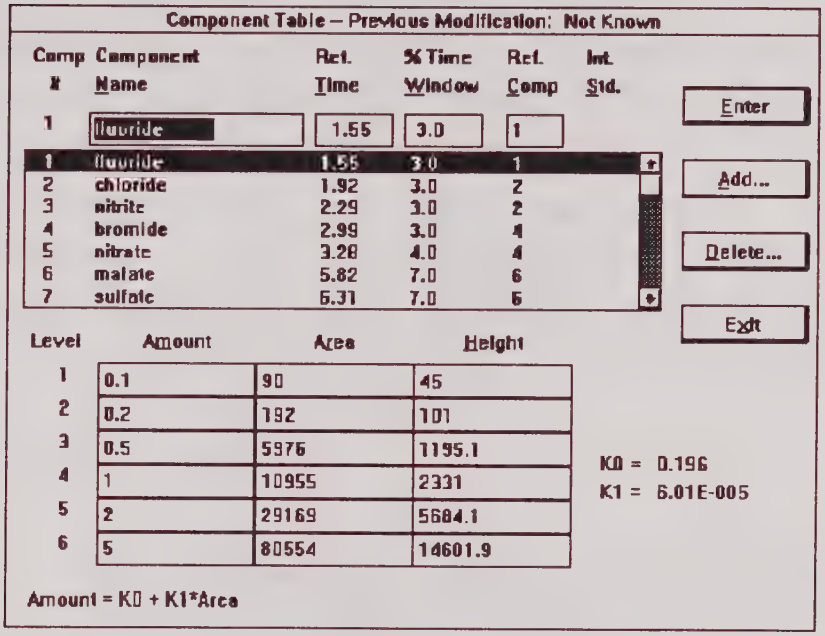


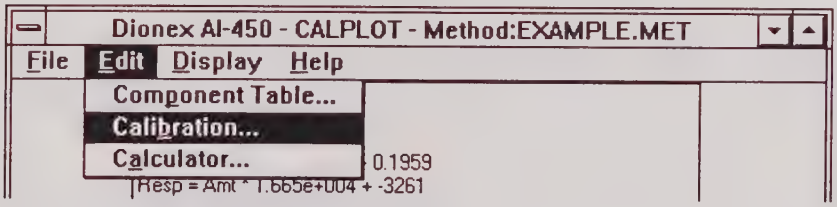


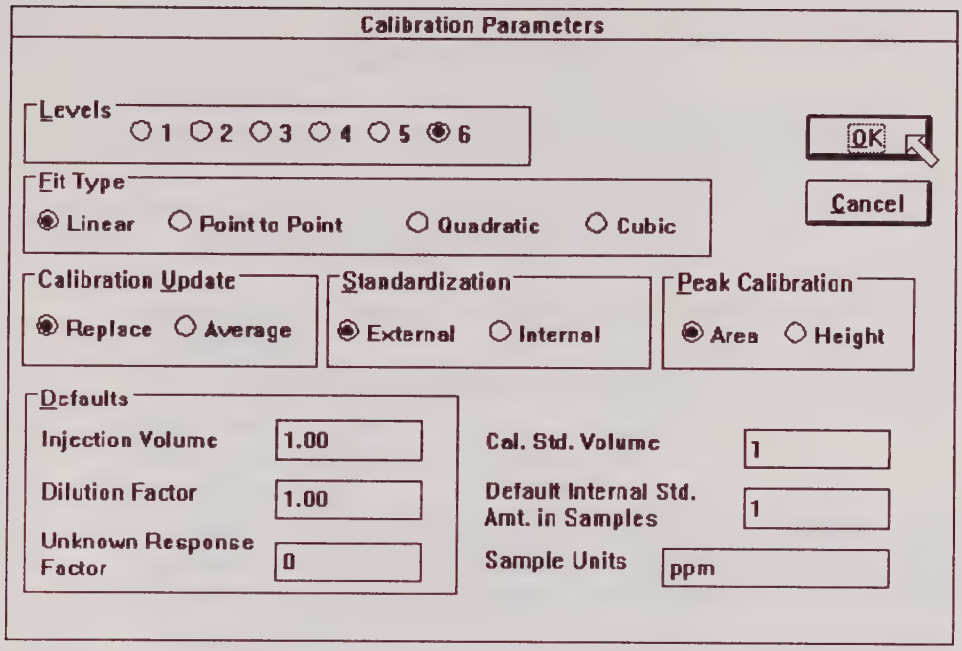
2. You can view all the calibration plots by scrolling through them with the scroll bar on the bottom of the window.

3. The Component table and the Calibration information can be edited from CALPLOT and then the method resaved.


Dionex AI-450 - CALPLOT - Method:EXAMPLE.MET
File
Edit
Display
Help
Component Table...
Calibration...
Calculator...
0.1959
Resp = Amt * 1.665e+004 + -3261

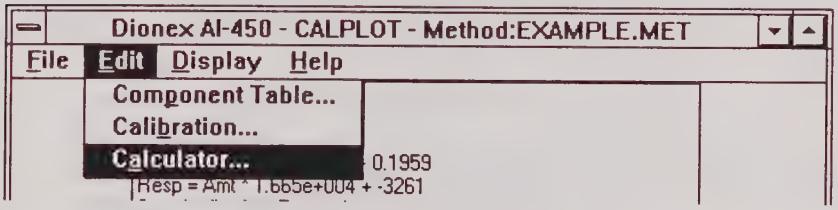

Component Table – Previous Modification: Not Known
Comp # Component Name
Ret. Time
% Time Window
Ret. Comp
Int. Std.
Enter
Add...
Delete...
Exit
1 fluoride 1.55 3.0 1
2 chloride 1.92 3.0 2
3 nitrite 2.29 3.0 2
4 bromide 2.99 3.0 4
5 nitrate 3.28 4.0 4
6 malate 5.82 7.0 6
7 sulfate 6.31 7.0 6
Level
Amount
Area
Height
1 0.1 90 45
2 0.2 192 101
3 0.5 5976 1195.1
4 1 10955 2331
5 2 29169 5684.1
6 5 80554 14601.9
K0 = 0.196
K1 = 6.01E-005
Amount = K0 + K1*Area

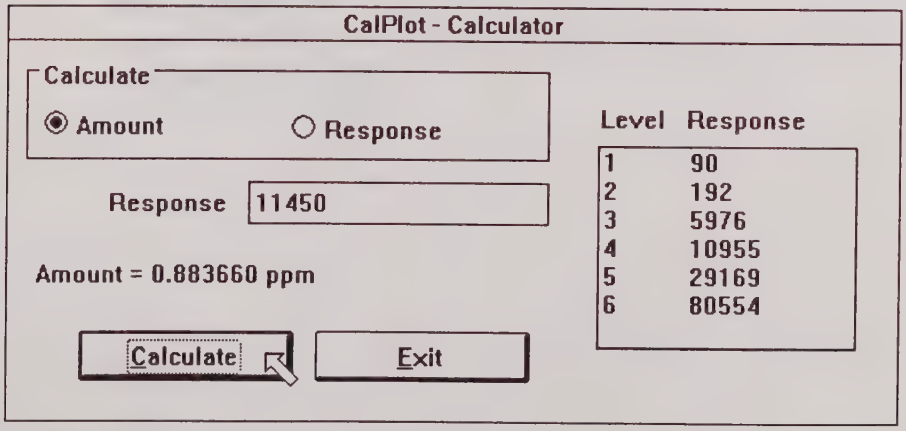

Dionex AI-450 - CALPLOT - Method:EXAMPLE.MET
File
Edit
Display
Help
Component Table...
Calibration...
Calculator...
0.1959
Resp = Amt * 1.665e+004 + -3261



B. Use of the "Calculator"

- There is a calculator function which can be used to calculate the amount of component from a response value or a response value from the amount of component. This calculation is based on the equation of the line that was determined for that component.





C. Using BATCH and CALPLOT (EXERCISE 10)

REPROCESSING CHROMATOGRAMS USING BATCH

A. Batch reprocess the calibration data files AI450CAL.D01 through AI450CAL.D05 using the 'OPTANION' method.

1. Build a batch schedule, select these five files, and save the selected files as "ANIONCAL".
2. View the schedule and change all the methods to "OPTANION" using copy in the Edit Menu.
3. Save this schedule again as "ANIONCAL".
4. Print this schedule.
5. In Processing Options, select "Update Methods from Autocal's" and "Restore Data After Reprocess" in order to store the integrated peak areas in "OPTANION" and optimize the integration of all the data files.
6. Start the batch process.
7. View the Calibration Plots for "OPTANION" using the CALPLOT program.

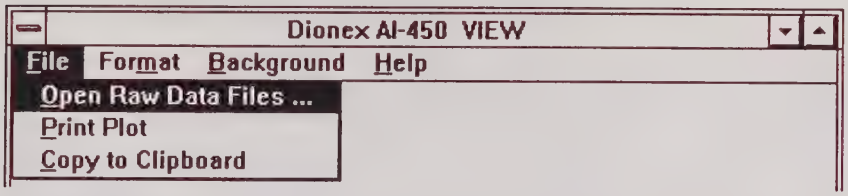
B. Batch reprocess the sample data files AI450SJW.D01-AI450SJW.D05 (San Jose tap water) or data files AI450SVW.D01-AI450SVW.D06 (Sunnyvale tap water) using the newly created calibration in method "OPTANION". These data files are replicate injections of undiluted tap water from San Jose or Sunnyvale, California, so a statistical summary can be generated within BATCH.

1. Build a batch schedule using one set of data files and save it as "ANIONH2O".
2. View the schedule and change all the methods to "OPTANION".
3. Save this schedule again as "ANIONH2O".
4. Print this schedule.
5. Select "View Statistical Summary" and "Print Statistical Summary" in the Processing Options.
6. Start the Batch process.

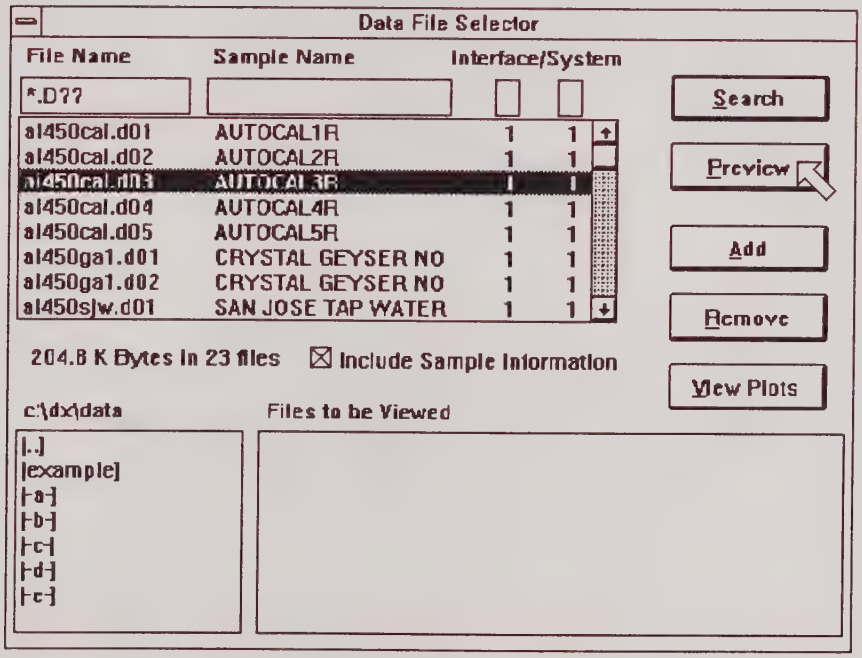
IX Viewing Multiple Chromatograms with VIEW

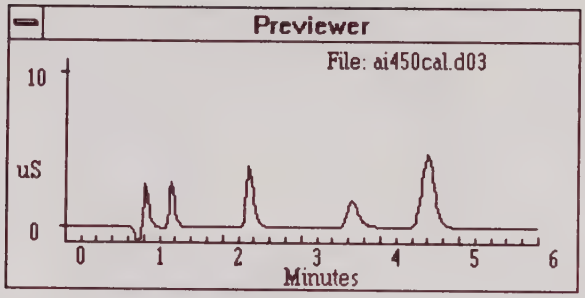
A. Previewing and Selecting Files

1. Select the "Open Raw Data Files" command from the the File Menu.

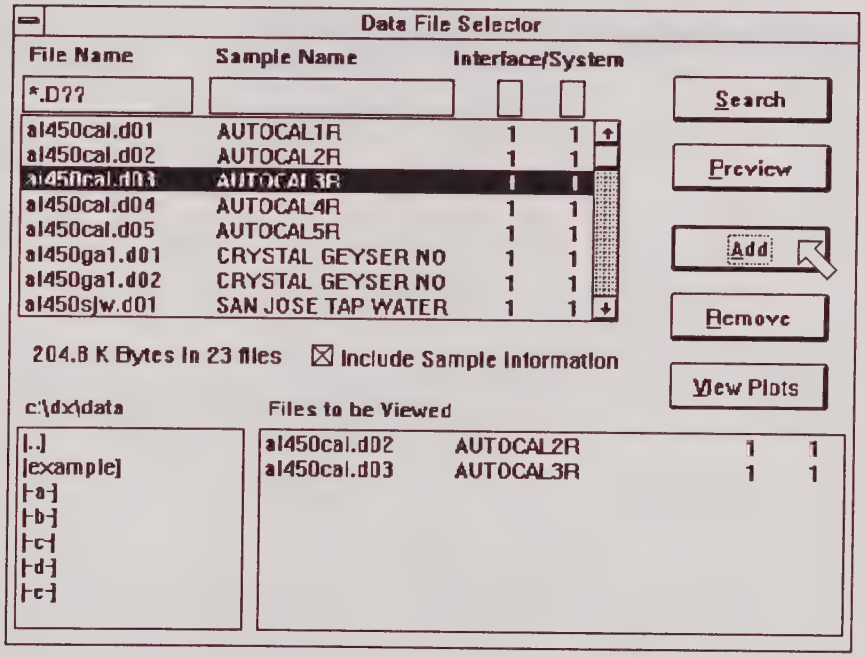


2. Highlighting a file and clicking on "Preview" allows you to look at the file before you add it.

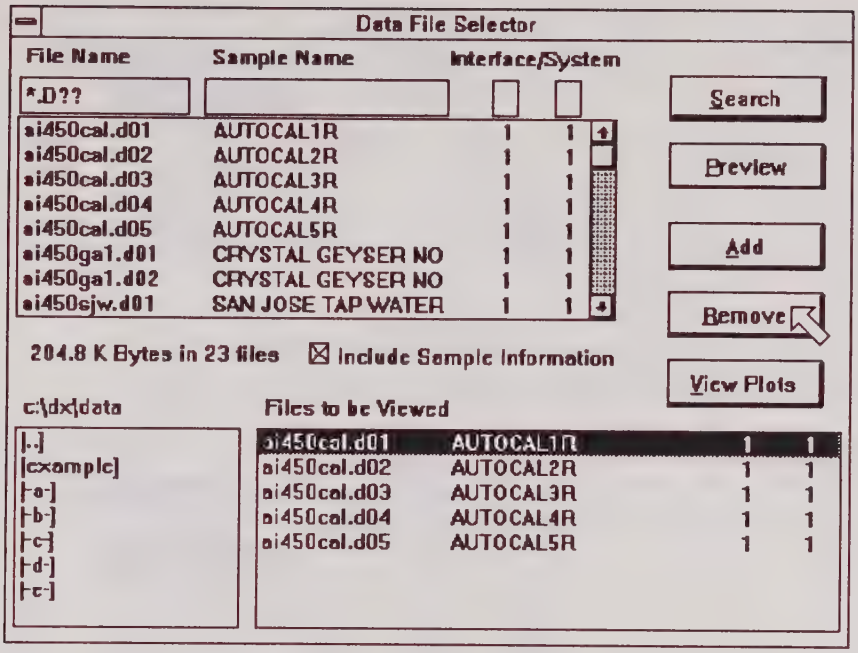




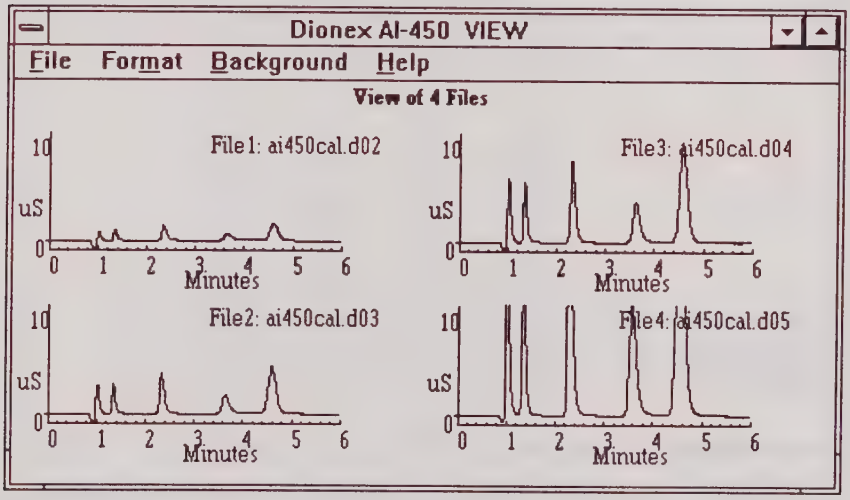
3. Select Files to be Viewed one at a time.



4. Remove a file from the list to be viewed by highlighting and clicking on the "Remove" button.

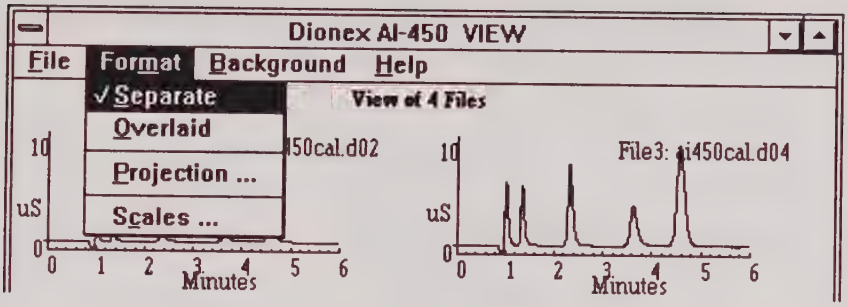


5. Click on the "View Plots" button to view the data files.

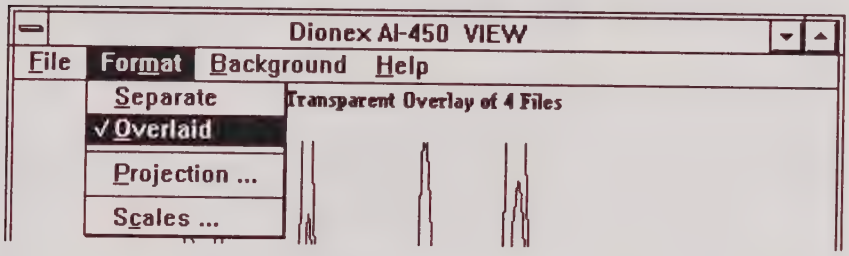


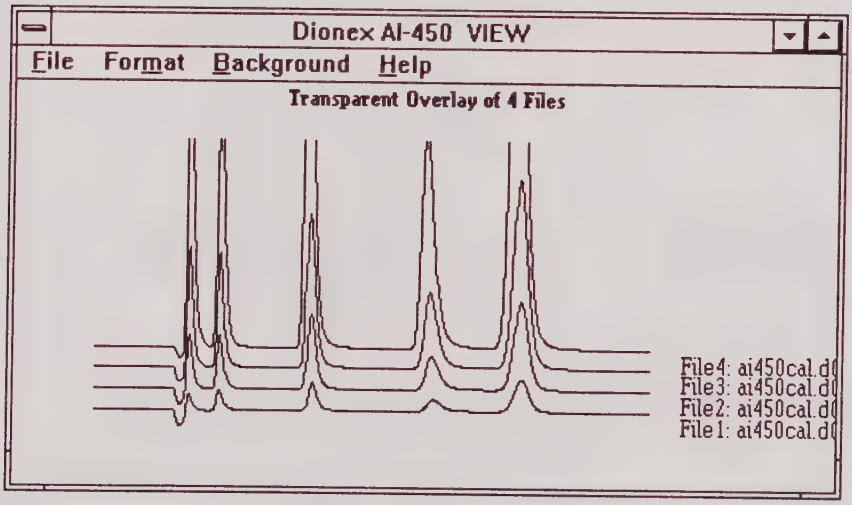
B. Changing the Viewing Format

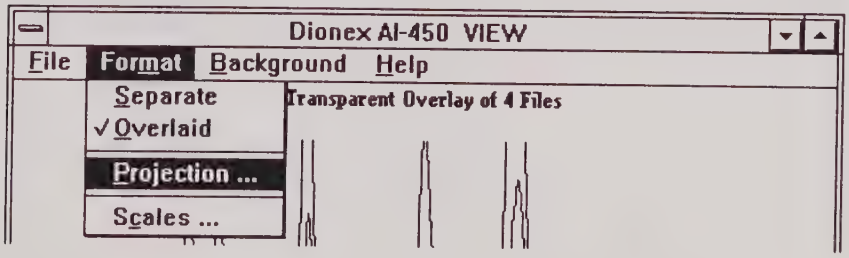
1. The "Separate" format plots the data files side-by-side and stacked individually to fill the window.



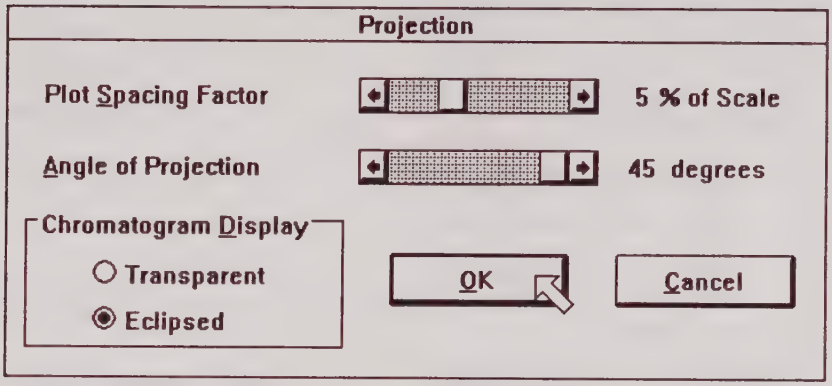
2. The "Overlaid" format plots the data files on top of each other, either as a transparent projection or as an eclipse (or offset in 3D).

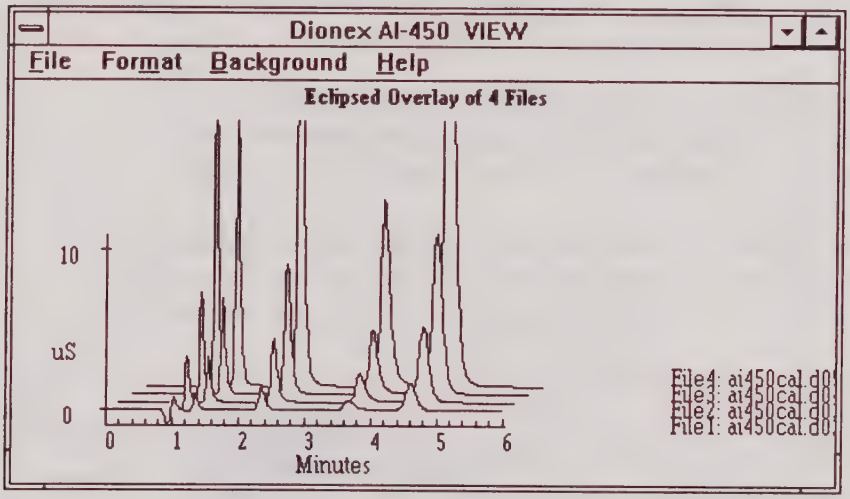




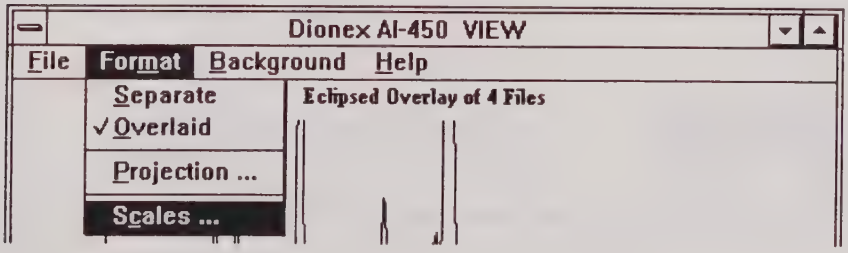


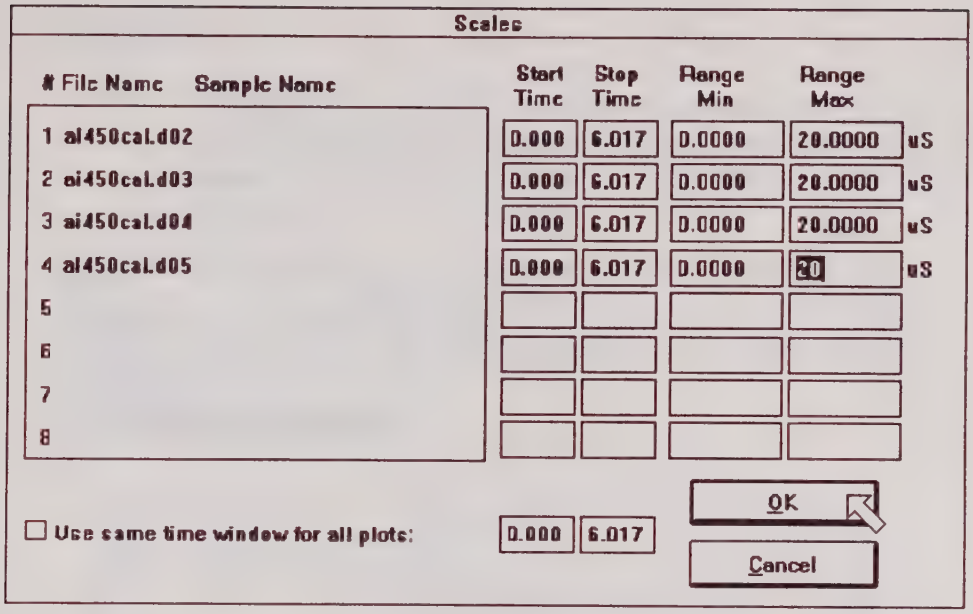
3. The Plot Spacing and the Angle of Projection of the Eclipsed Projection can be adjusted to achieve the most desirable "3D effect".





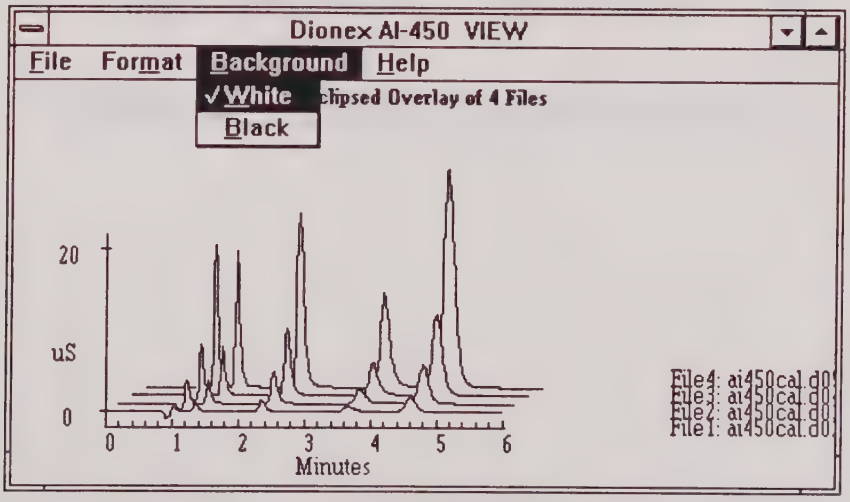
4. The Scales can be changed to fit all the peaks on the plot, or view any portion of the plot in more detail.





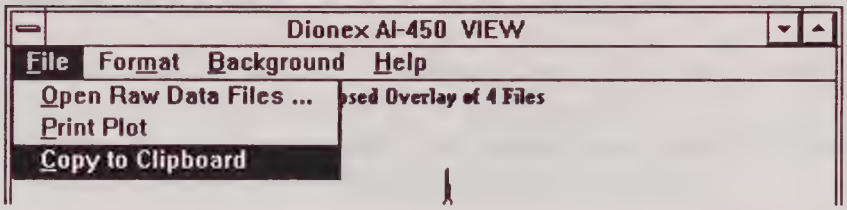
- If the "Use same time window for all plots" option is chosen, the individual time settings cannot be changed. The eclipse plot ALWAYS uses the same time window for all plots.

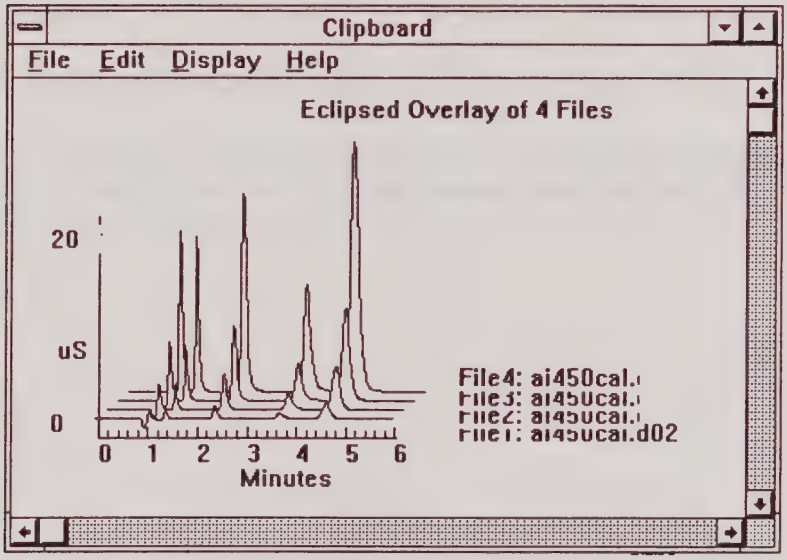
5. The Background of the plot on the screen can be set to be either White or Black, but DO NOT try to print a plot with a black background or you will get a page full of ink!



C. Exporting

1. The completed plot can be printed directly to the printer or copied to the clipboard to be imported as a scaled graphics file into programs which can accept such files (e.g Microsoft Write, Aldus Pagemaker).





EXERCISE 11

DISPLAYING MULTIPLE DATA FILES USING VIEW

A. Create a 3-D projected view of data files AI450CAL.D02 through AI450CAL.D05.

1. Select the desired files and, if necessary, check them using "PREVIEW".
2. Choose the "Overlaid" mode in the Format menu.
3. Choose the "Projection" mode in the Format menu, select "Eclipsed" and adjust the spacing and angle to give the best 3D effect.

B. Print this plot.

C. Copy this plot to the Clipboard using the command in the File menu.

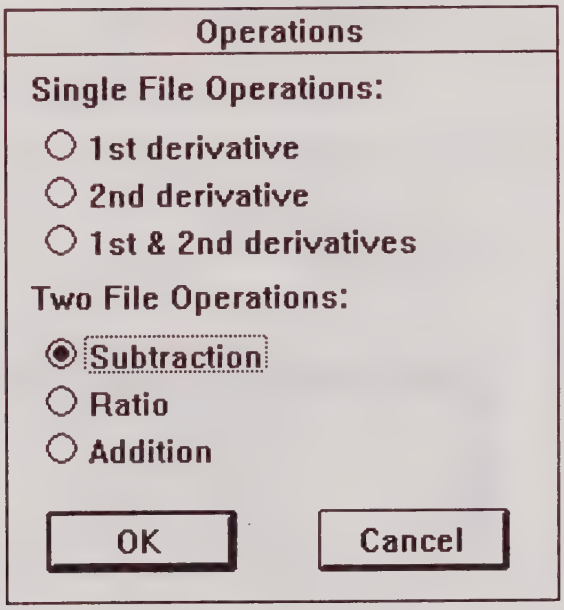
D. Start the Clipboard program from the icon in the Program Manager and see that the plot is there. Close the Clipboard program when finished - the plot will remain in the "Clipboard memory".

X DATAMATH and When is it Used?

A. What Does the Program DO?

- DATAMATH performs mathematical operations on one or two data files to generate a "Result File"
- The most common use of DATAMATH is to subtract a blank run from a sample run.

B. Selecting Mathematical Operation



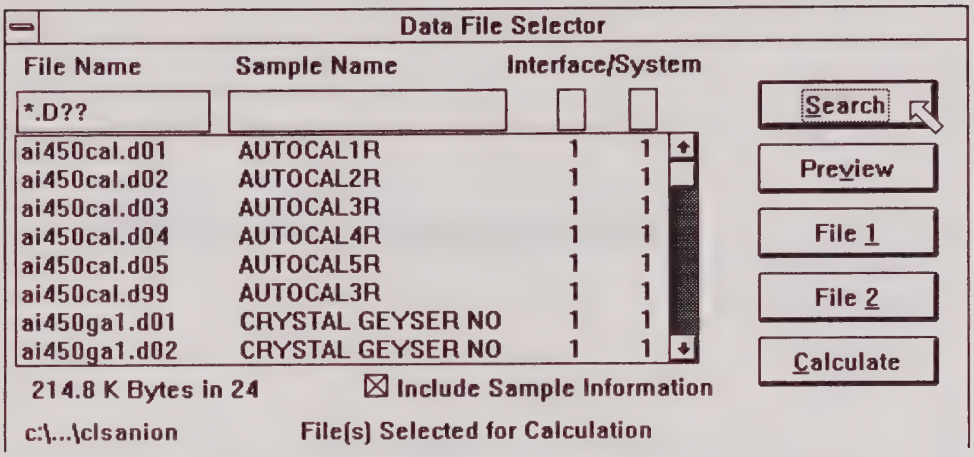
1. Two File Manipulations

   - Subtraction
   - Ratio
   - Addition

2. One File Manipulations

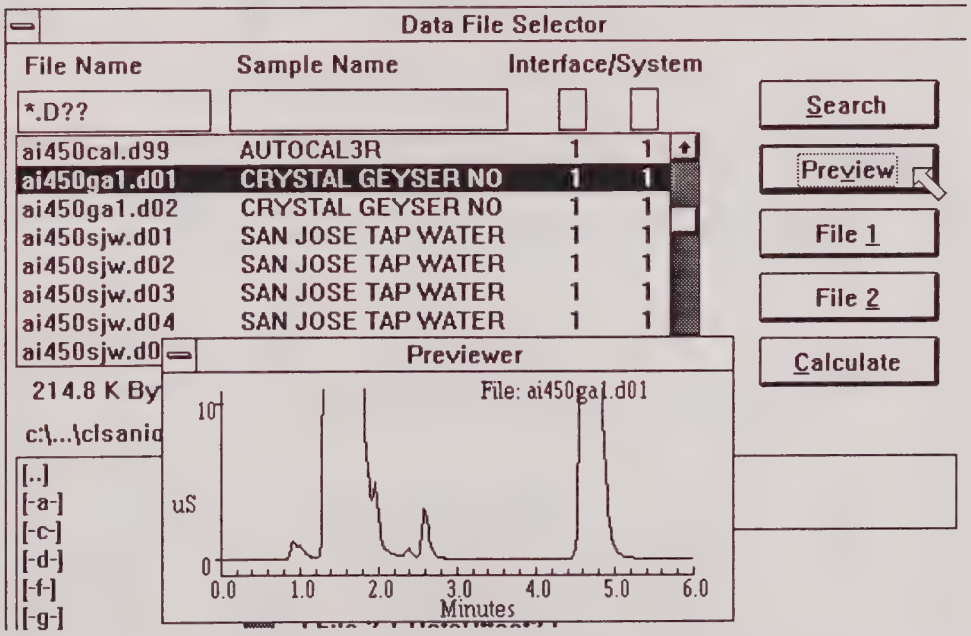
   - Derivatives

C. Selecting Files

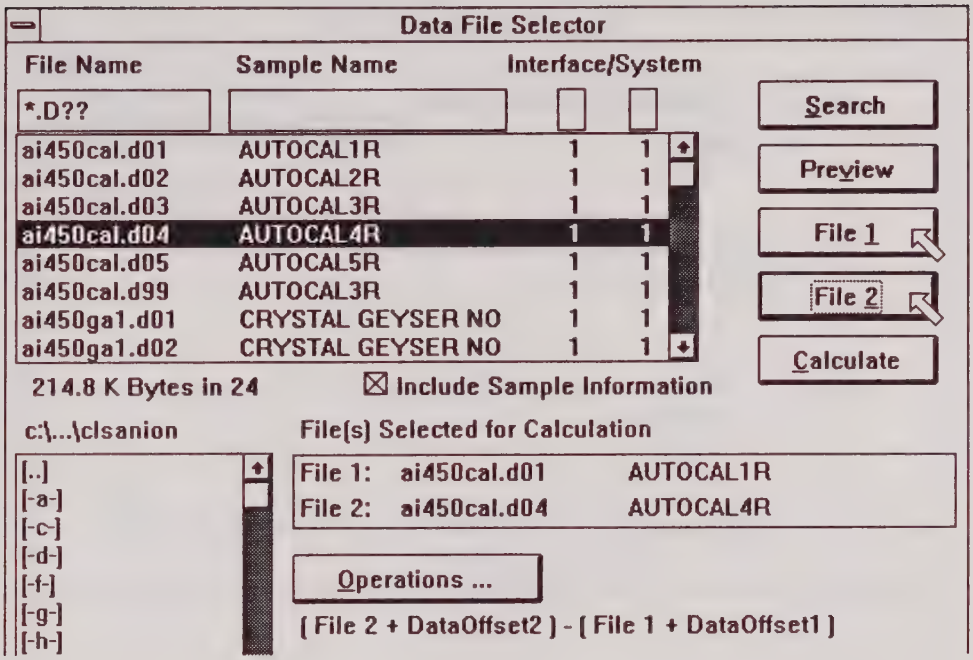


1. Search directories for data files

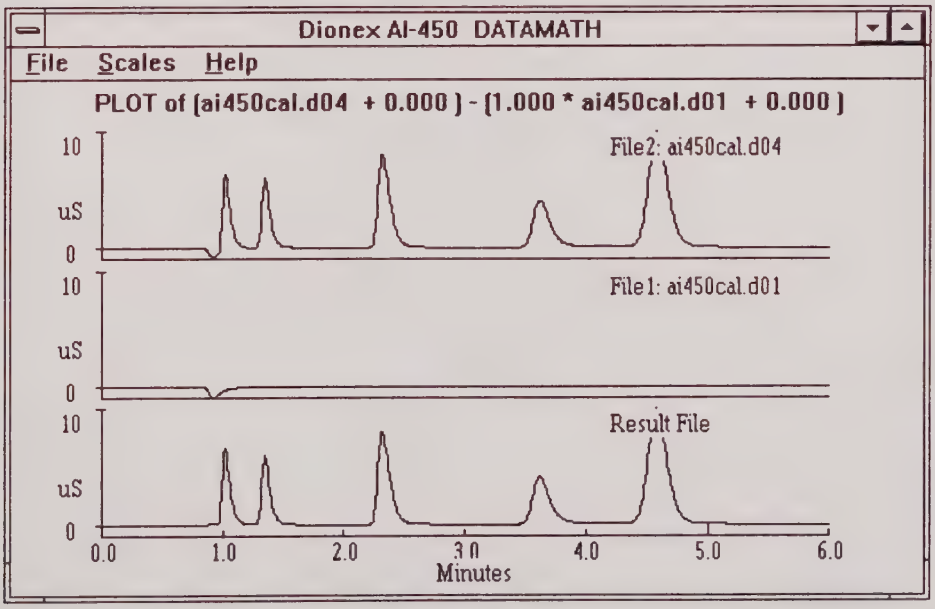
2. Preview chromatograms quickly to refresh your memory



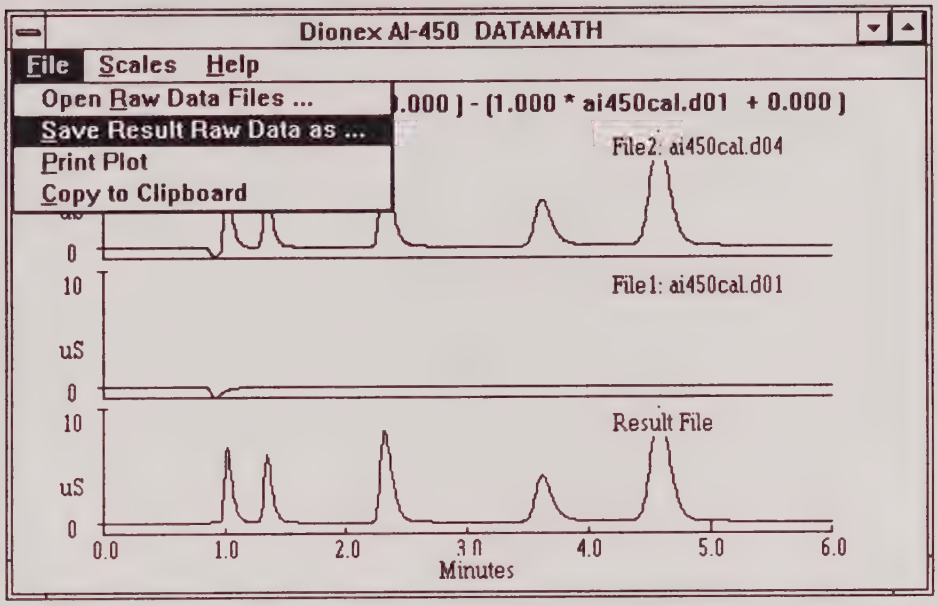
3. Select File 1 and File 2 to do the calculations



4. Press the **Calculate** button to perform the Calculation.

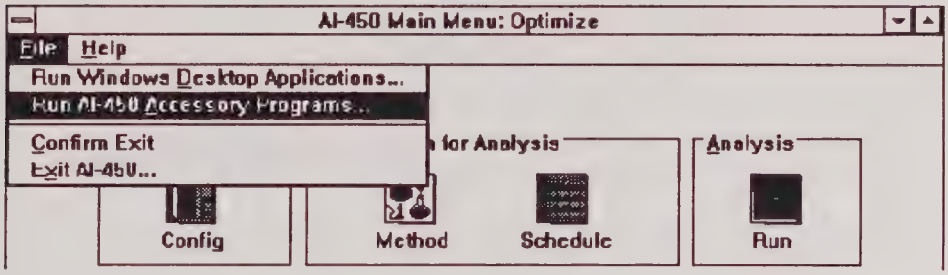


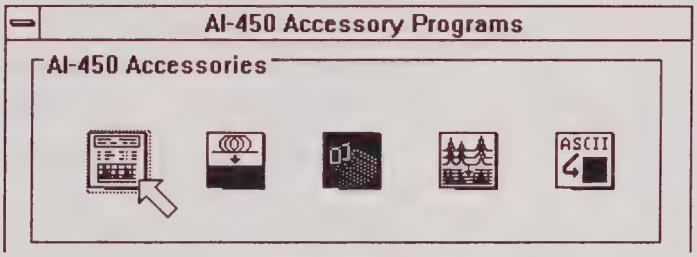
5. Save Result File, if desired.

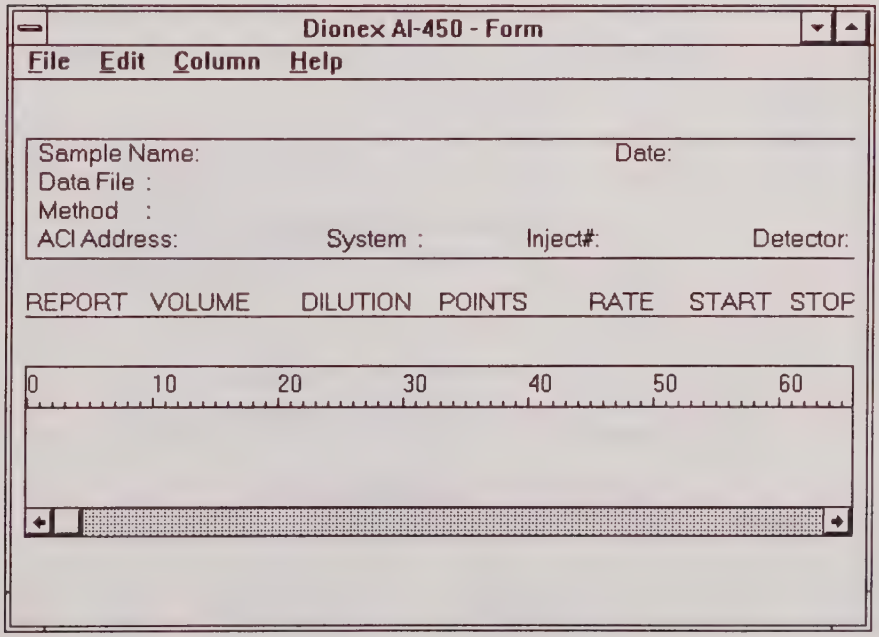


XI Customizing Reports with FORM (Optional)

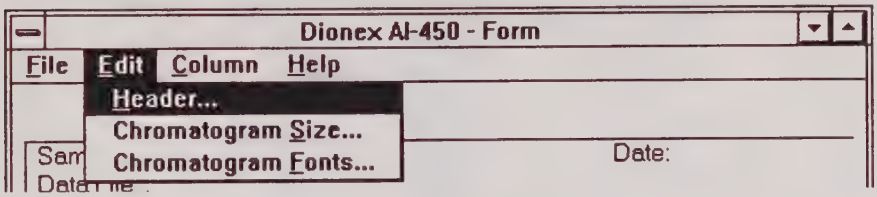
A. The FORM program can be accessed from the "Run AI-450 Accessory Programs" command of the MainMenu File Menu.

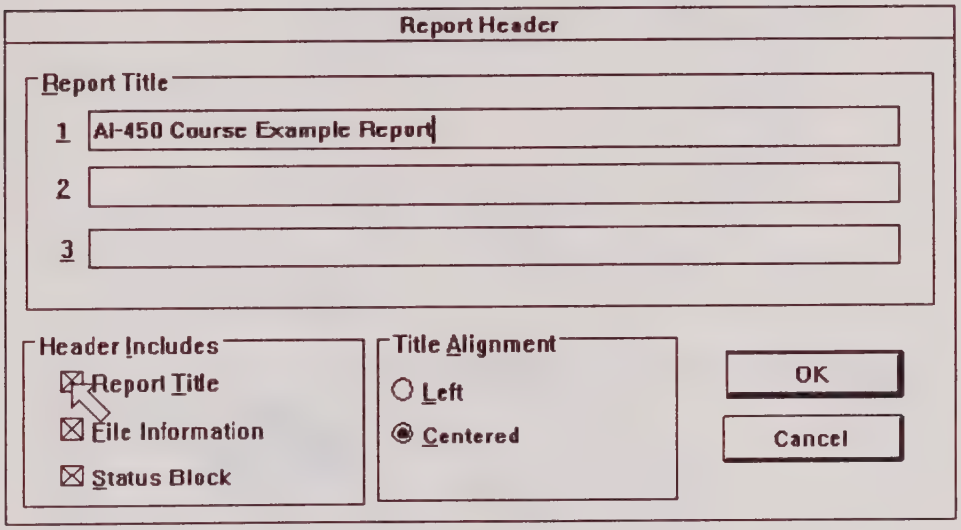




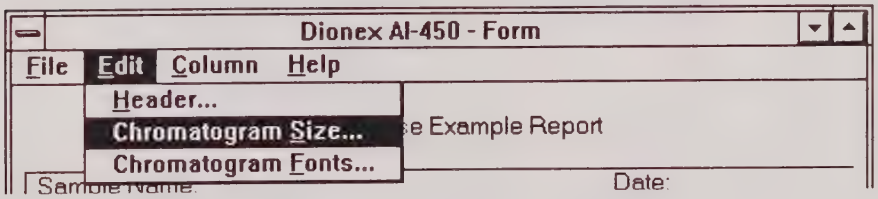


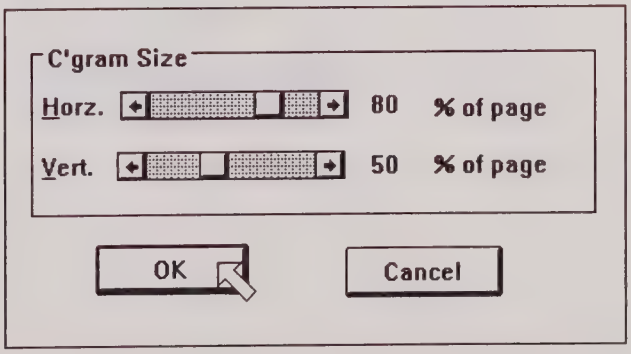
B. The FORM program can be used to create unique titles and header information for your reports.

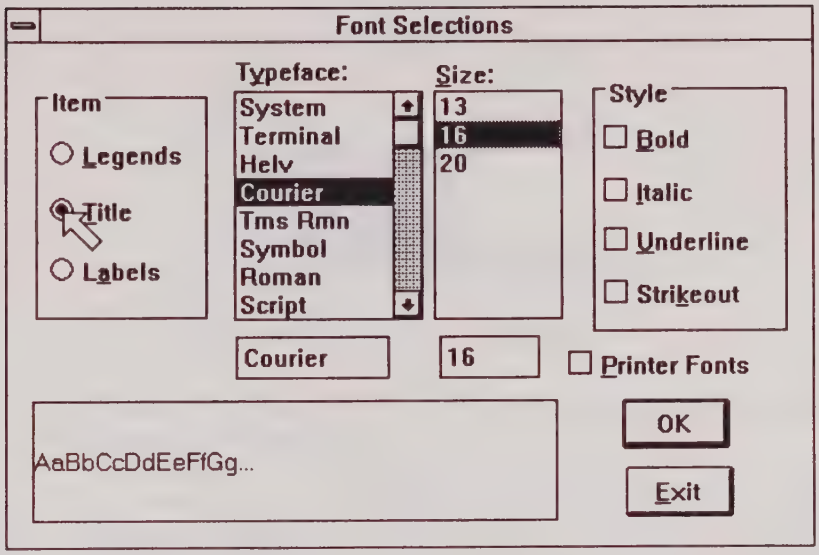




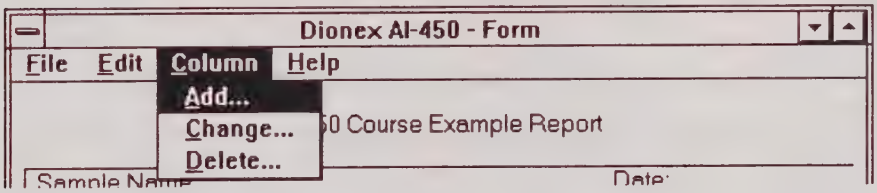
C. Through the Edit Menu, you can change the size of the printed chromatogram and the type of fonts on the chromatogram.

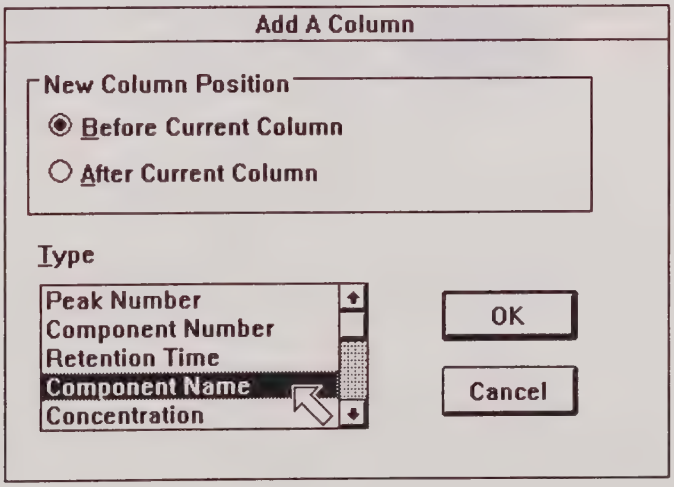


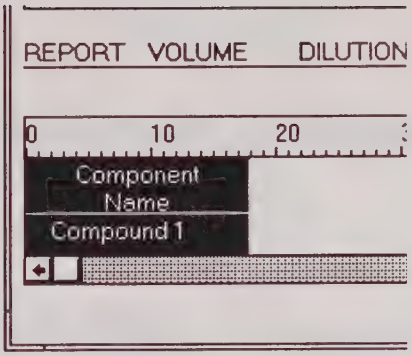




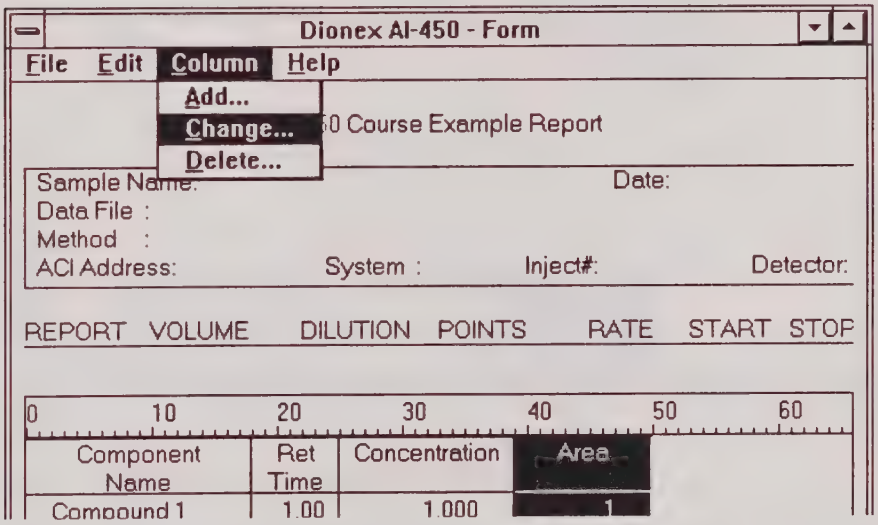
D. Through the Column Menu, you can select exactly the information you need in the body of the report.

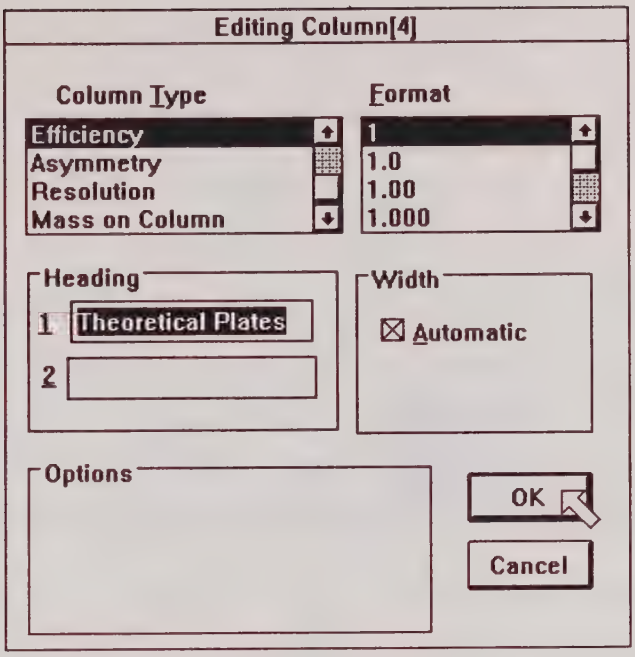


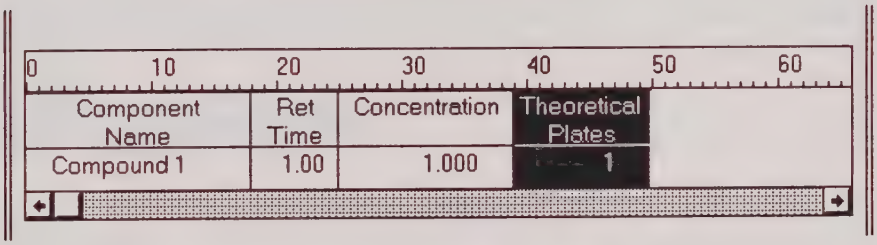




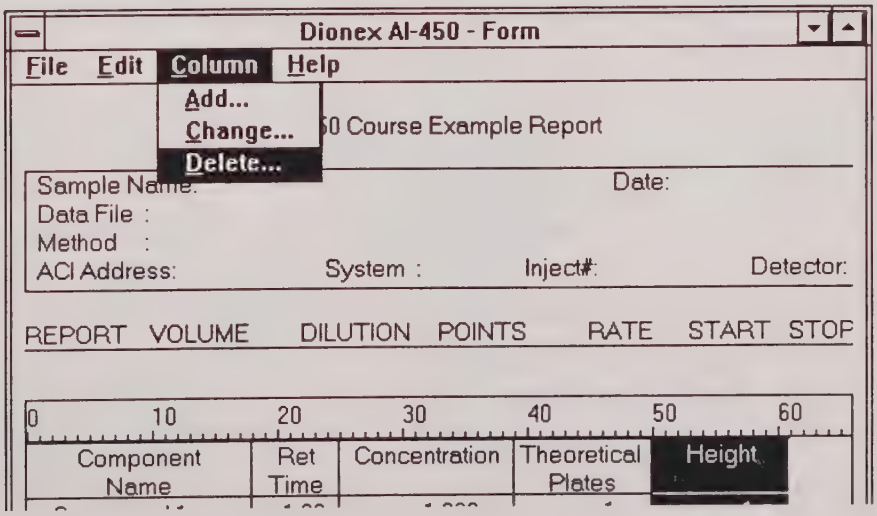
E. You can change existing columns to another parameter and even customize what the parameter is called.

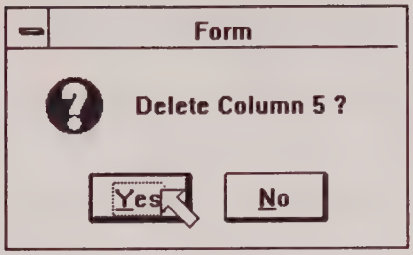


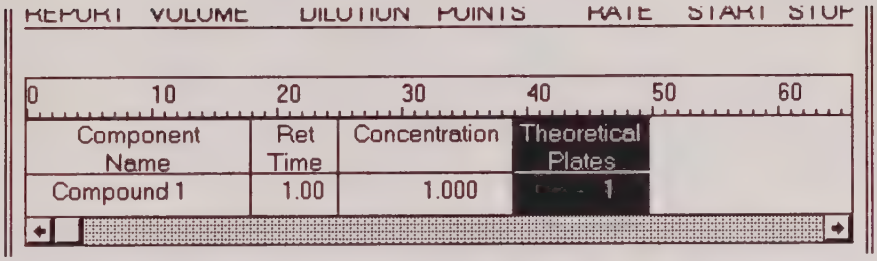




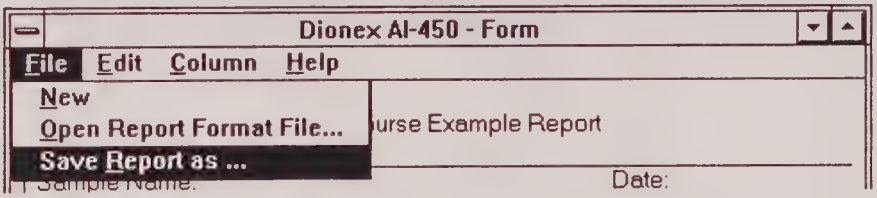
F. Unwanted parameters can be easily deleted.

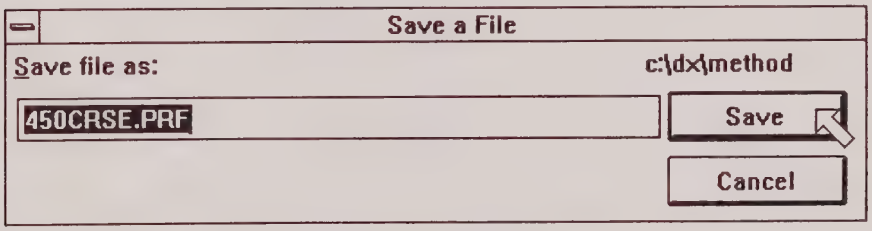


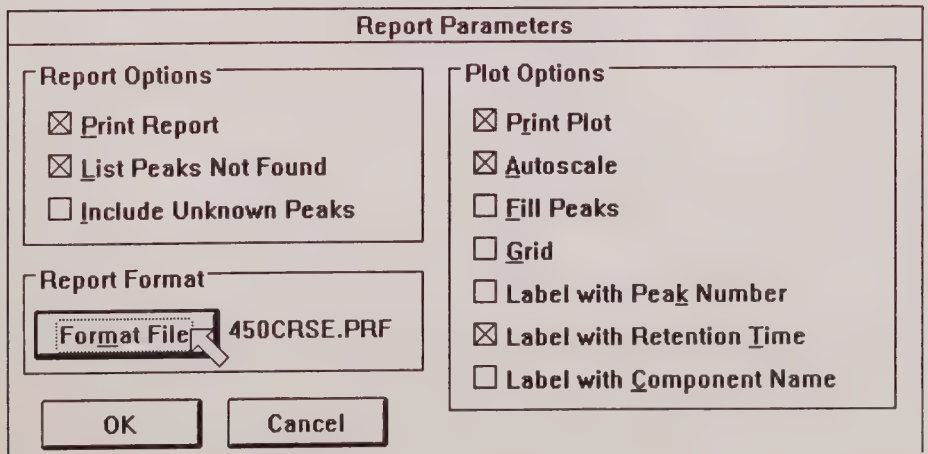




G. The customized report format can be saved for later inclusion in the Method.







FORM EXERCISE (Optional)

A. Using the FORM program, create a customized report format having the following characteristics:

1. Give the header the title of "AI-450 Course Example Report" and center it.
2. Scale the chromatogram to occupy 80% of the horizontal dimension and 50% of the vertical dimension.
3. Specify a 16pt Courier font for the chromatogram title.
4. Select the following columns for the body of the report: Component name, retention time, concentration, efficiency (change the name "Efficiency" to "Theoretical Plates").

B. Save this customized report format as "450CRSE.PRF" in the Method subdirectory of DX.

C. Using the OPTIMIZE program, open one of the water sample data files, specify the 450CRSE.PRF report format in the method, and print out a report to verify that the format is correct.

Alltech Associates, Inc. / Varex Group
4000 Blackburn Lane • Burtonsville, Maryland 20866
Phone: 301-421-1616 • Fax: 301-421-1882

ELSD MK III

Dear Customer,

The Varex EVAPORATIVE LIGHT SCATTERING DETECTOR is a delicate scientific instrument. Please retain the original carton and inner packing pieces for any future shipping or transport needs.

Should you need to return the unit to Varex for service, please ship it in the inner box without the large outer carton.

(It is not necessary to send back any accessories, i.e., power cords, exhaust kit, tools, etc.)

Thank you.

PACKING INSTRUCTIONS FOR THE ELSD MK III

1. Cover the Nebulizer inlet (at the top of the unit) to prevent internal contamination of the Nebulizer.

2. Close the stainless-steel doors and secure them in place with a piece of adhesive tape.

[illegible] and tie off the bag opening. (Try to

DIONEX
1228 Titan Way
Sunnyvale, CA 94086 USA
(408) 737-0700
Telex: 348347
Cable: Dionex Sunnyvale